The Portable Extensible Toolkit for Scientific Computing

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Houston, TX Oct 31, 2016

Main Point

Never believe *anything*,

unless you can run it.

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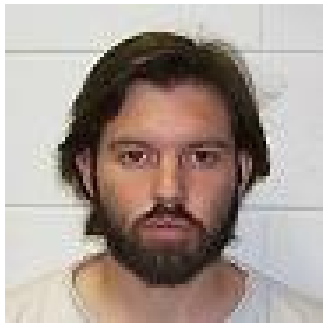
unless you can run it.

Outline

The PETSc Team


Matt Knepley


Barry Smith


Satish Balay


Hong Zhang


Jed Brown


Lisandro Dalcin


Stefano Zampini


Mark Adams


Toby Issac

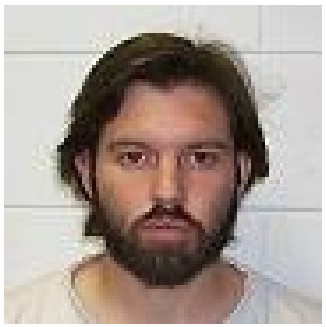
Collaborators


Barry Smith


Jay Bardhan


Boyce Griffith


Jed Brown


Matt Knepley


Michael Lange


Brad Aagaard


Mark Adams


Toby Issac

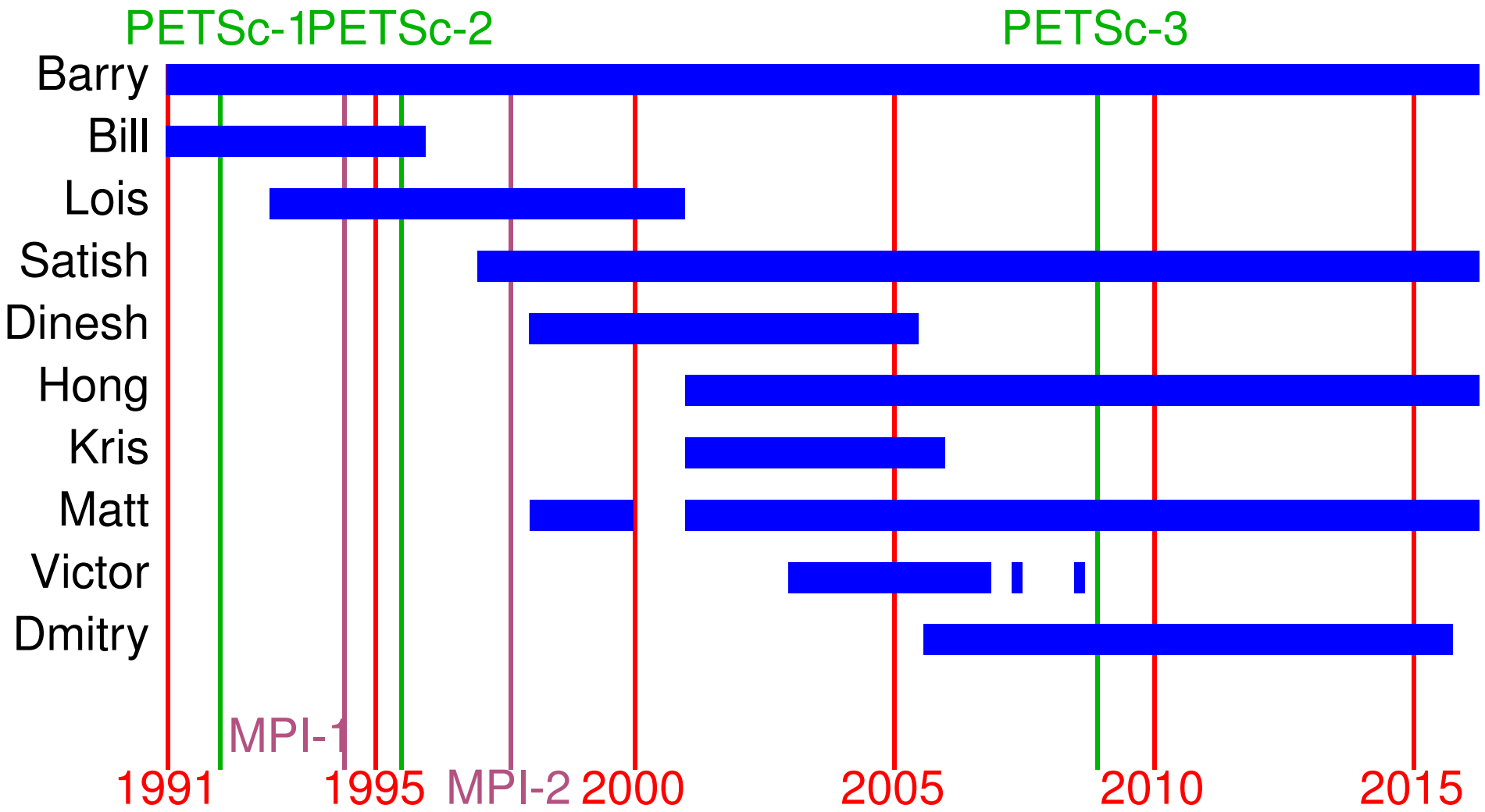
Collaborators (Degree)

Math	**EE**	**Math**
Barry Smith	Jay Bardhan	Boyce Griffith
Geo	**CS**	**CS**
Jed Brown	Matt Knepley	Michael Lange
CivE	**CivE**	**CSE**
Brad Aagaard	Mark Adams	Toby Issac

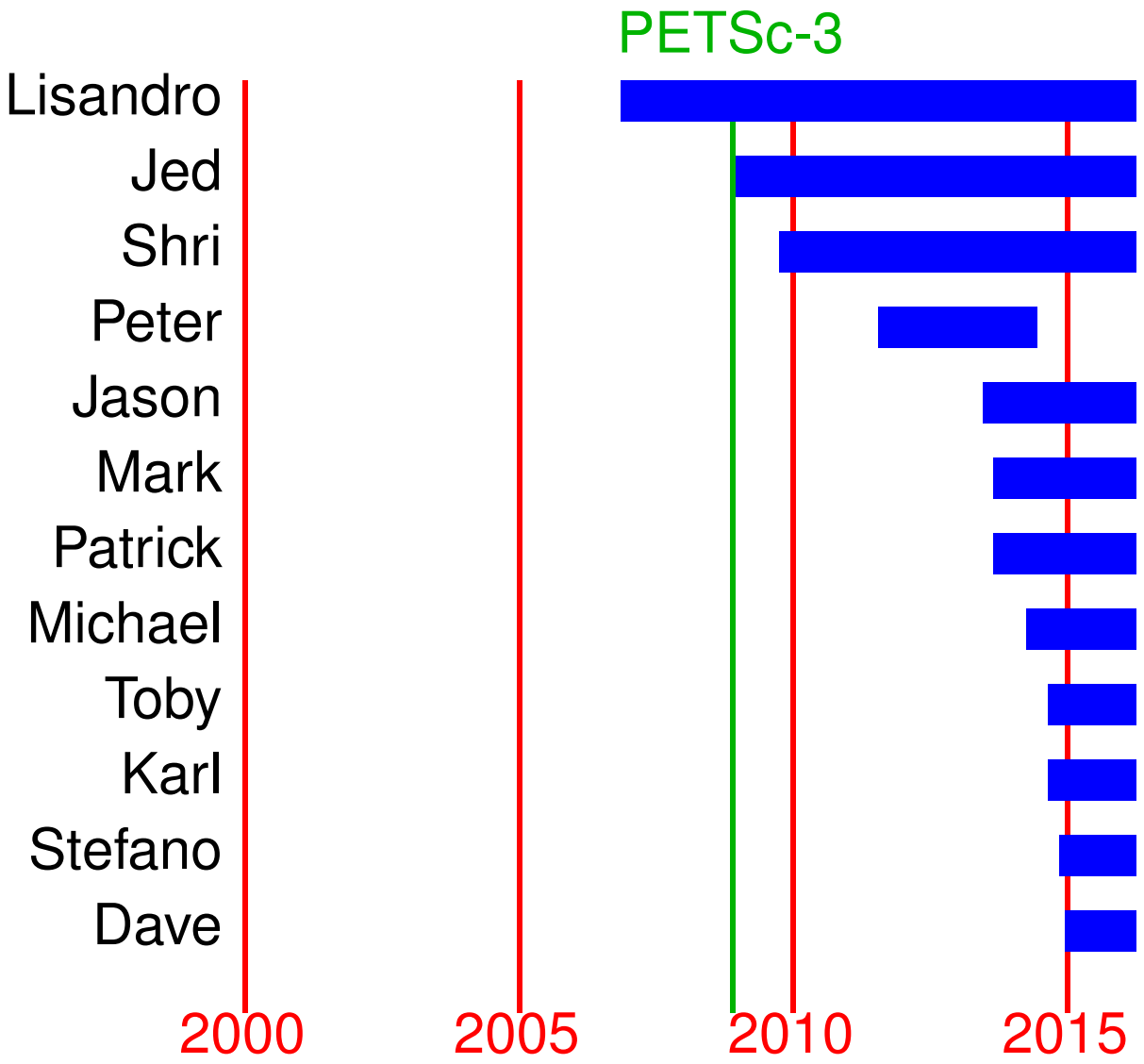
Collaborators (Occupation)

MCS	**MechE**	**Math/Med**
Barry Smith	Jay Bardhan	Boyce Griffith
CS	**Math**	**Geo**
Jed Brown	Matt Knepley	Michael Lange
USGS	**Math**	**CS**
Brad Aagaard	Mark Adams	Toby Issac

Timeline (Old People)



Timeline (Young People)

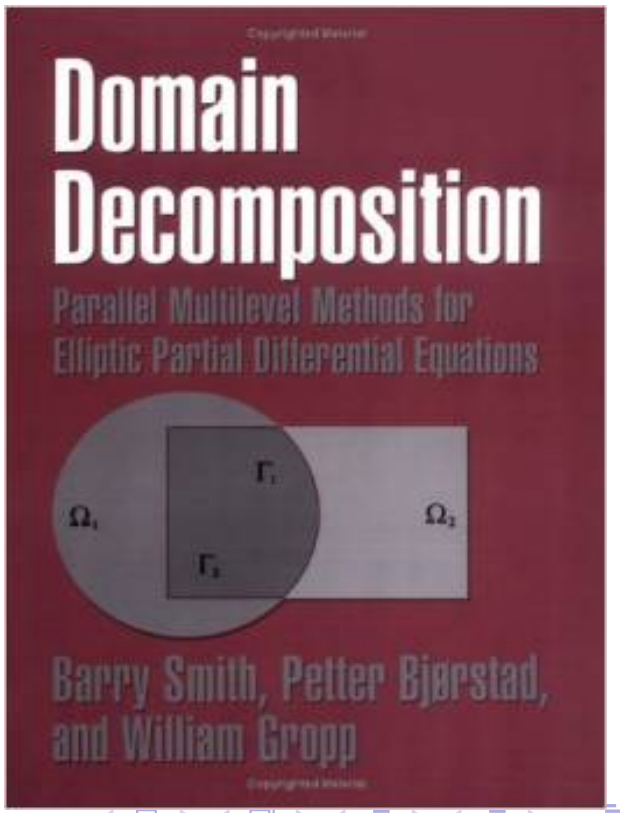


How did PETSc Originate?

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
    - ECP, AMR Program, SciDAC, MICS Program, INL Reactor Program
  - National Science Foundation
    - SI2, CIG, CISE, Multidisciplinary Challenge Program
  - Intel Parallel Computing Center

What is PETSc?

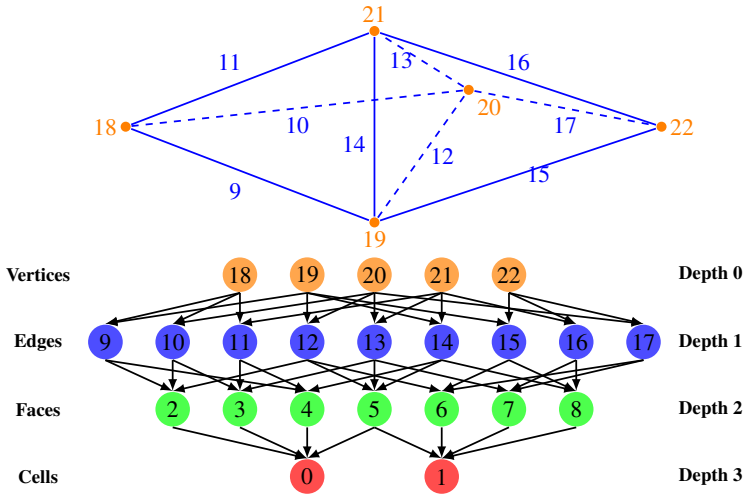
PETSc is one of the most popular software libraries in scientific computing.

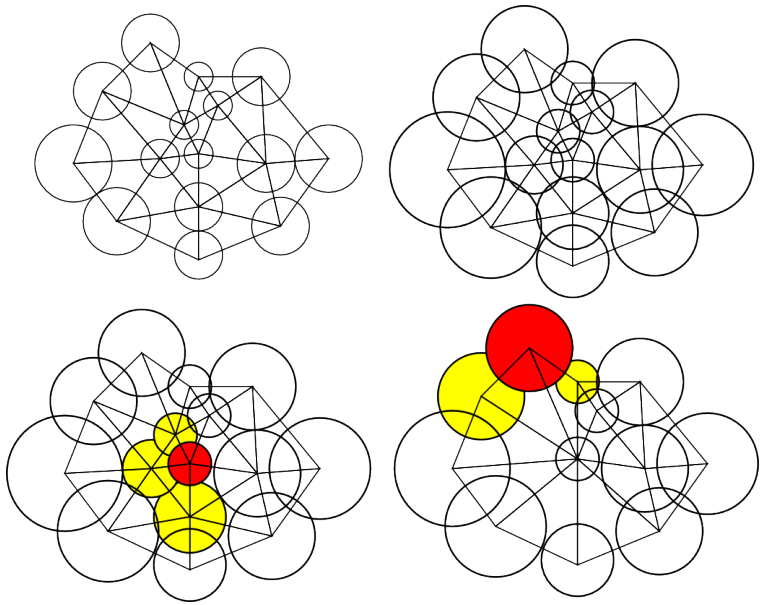
As a principal architect since 2001, I developed

- unstructured meshes (model, algorithms, implementation),
- nonlinear preconditioning (model, algorithms),
- FEM discretizations (data structures, solvers optimization),
- optimizations for multicore and GPU architectures.

What is PETSc?

Knepley, Karpeev, Sci. Prog., 2009. Brune, Knepley, Scott, SISC, 2013.





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Brune, Knepley, Smith, and Tu, SIAM Review, 2015.

Type	Sym	Statement	Abbreviation
Additive	$+$	$\vec{x} + \alpha(\mathcal{M}(\mathcal{F}, \vec{x}, \vec{b}) - \vec{x}) + \beta(\mathcal{N}(\mathcal{F}, \vec{x}, \vec{b}) - \vec{x})$	$\mathcal{M} + \mathcal{N}$
Multiplicative	$*$	$\mathcal{M}(\mathcal{F}, \mathcal{N}(\mathcal{F}, \vec{x}, \vec{b}), \vec{b})$	$\mathcal{M} * \mathcal{N}$
Left Prec.	$-_L$	$\mathcal{M}(\vec{x} - \mathcal{N}(\mathcal{F}, \vec{x}, \vec{b}), \vec{x}, \vec{b})$	$\mathcal{M} -_L \mathcal{N}$
Right Prec.	$-_R$	$\mathcal{M}(\mathcal{F}(\mathcal{N}(\mathcal{F}, \vec{x}, \vec{b})), \vec{x}, \vec{b})$	$\mathcal{M} -_R \mathcal{N}$
Inner Lin. Inv.	$\backslash$	$\vec{y} = \vec{J}(\vec{x})^{-1}\vec{r}(\vec{x}) = \mathsf{K}(\vec{J}(\vec{x}), \vec{y}_0, \vec{b})$	$\mathcal{N} \backslash \mathsf{K}$

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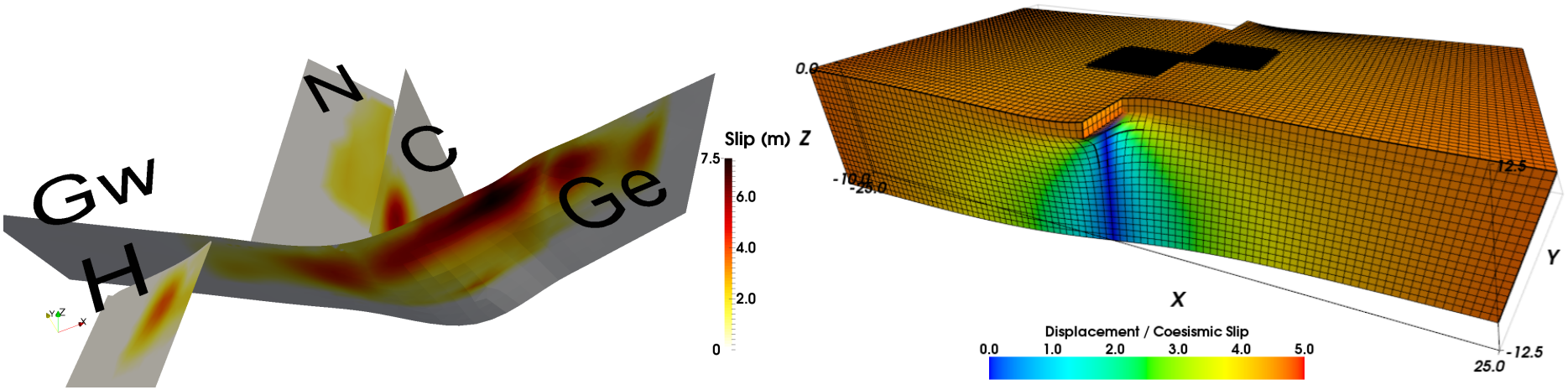
Aagaard, Knepley, and Williams, J. of Geophysical Research, 2013.



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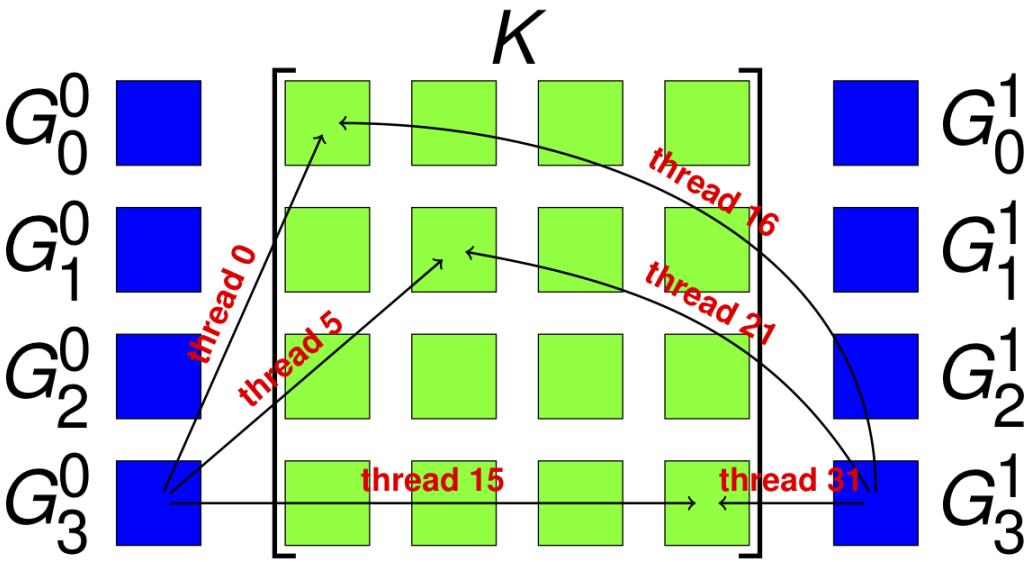
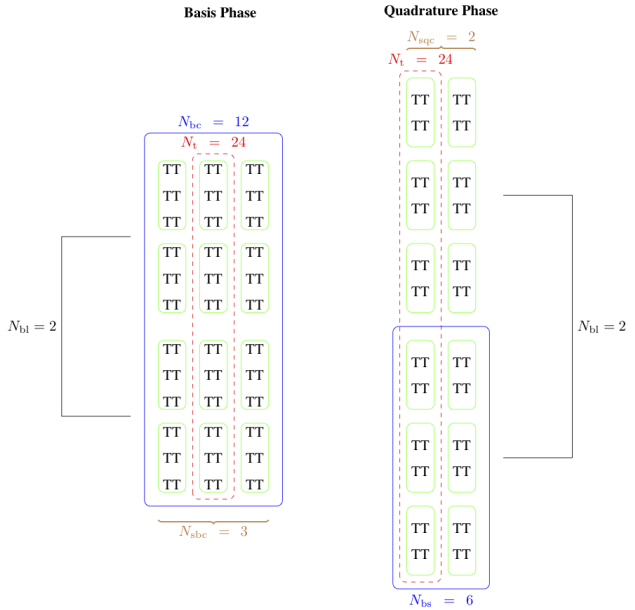
Knepley and Terrel, Transactions on Mathematical Software, 2012.





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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
  - 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 1,500,000 cores efficiently
  - Gordon Bell Prize Mantle Convection on IBM BG/Q Sequoia
- PETSc applications have run at 23% of peak (600 Teraflops)
  - Jed Brown on NERSC Edison
  - HPGMG code

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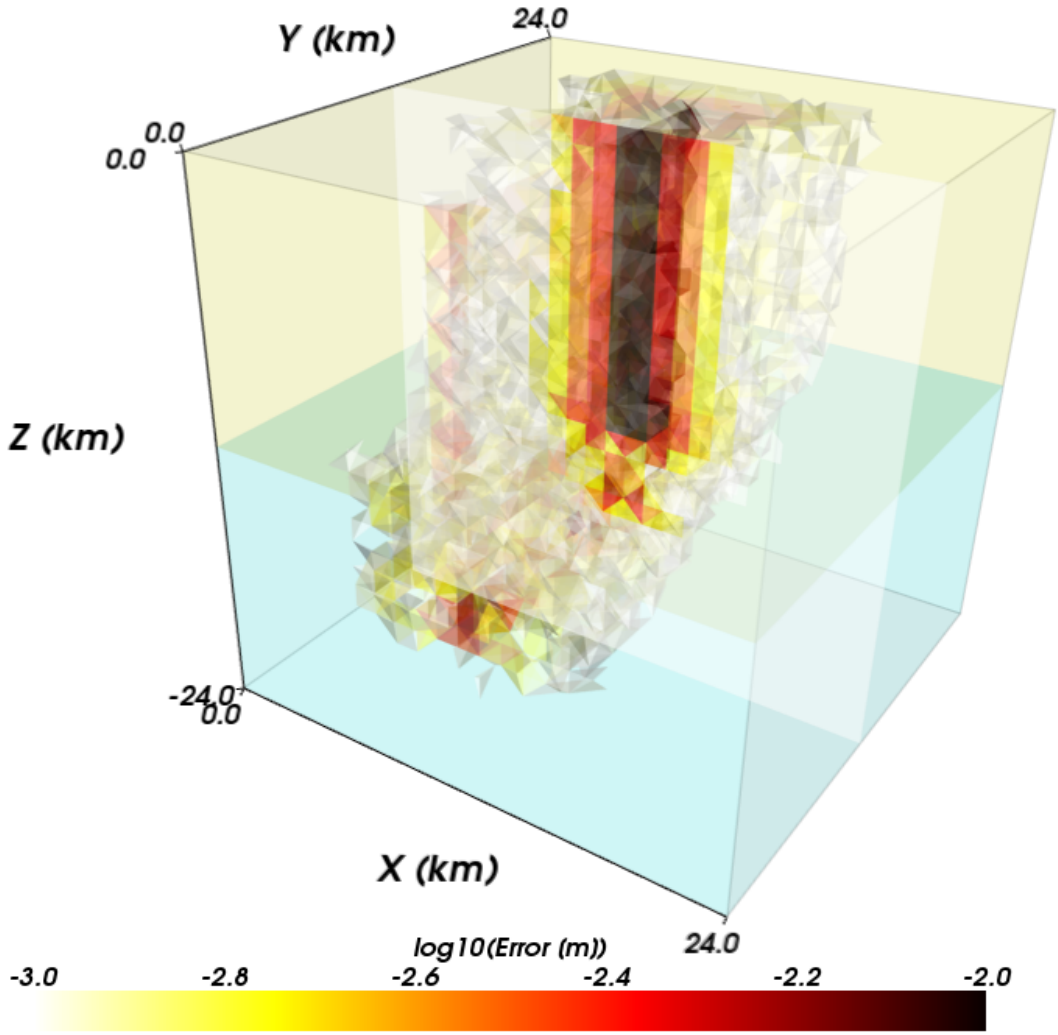
PyLith

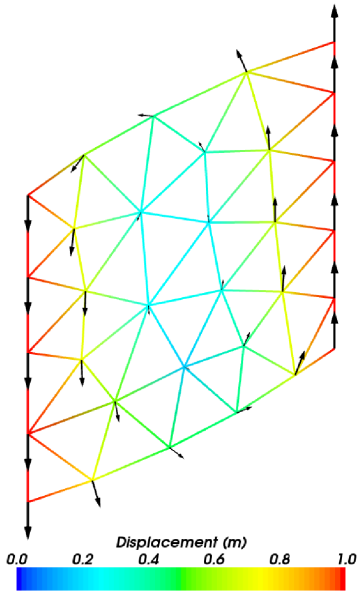
- Multiple problems
  - Dynamic rupture
  - Quasi-static relaxation
- Multiple models
  - Nonlinear visco-plastic
  - Finite deformation
  - Fault constitutive models
- Multiple meshes
  - 1D, 2D, 3D
  - Hex and tet meshes
- Parallel
  - PETSc solvers
  - DMPlex mesh management

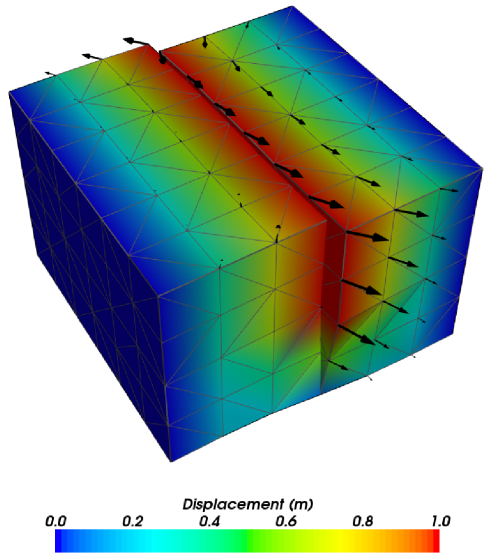


[a] Aagaard, Knepley, Williams

Multiple Mesh Types

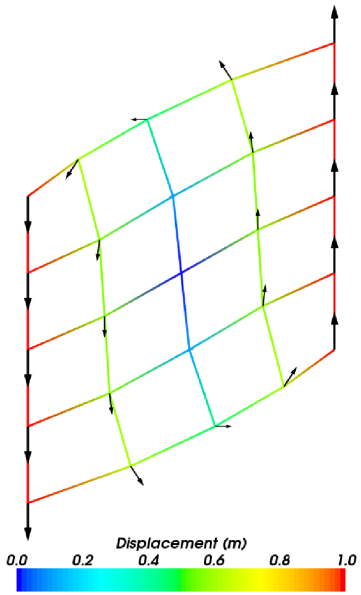
Triangular

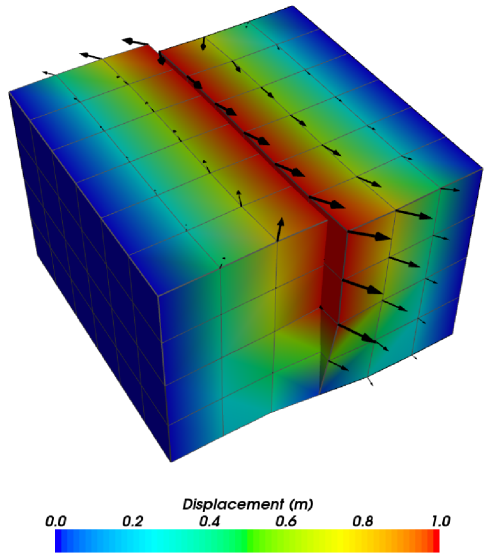




Tetrahedral

Rectangular

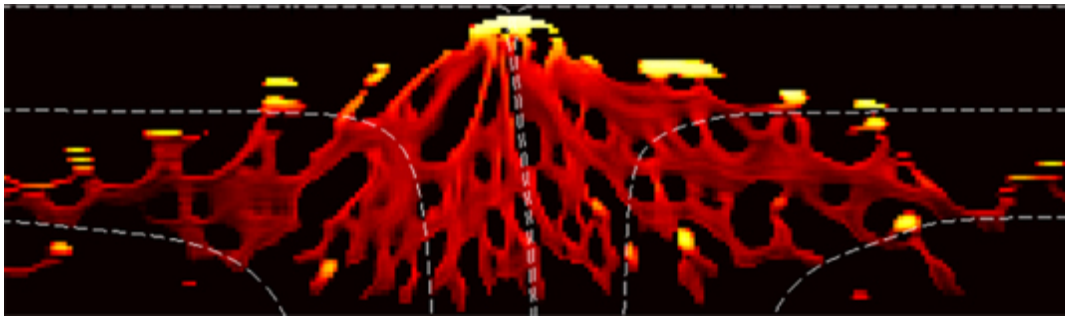


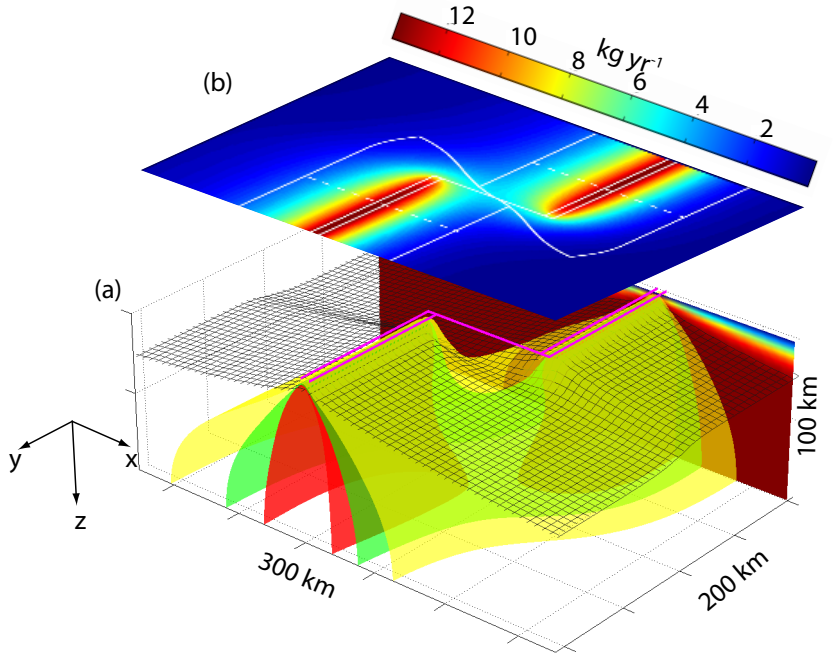


Hexahedral

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

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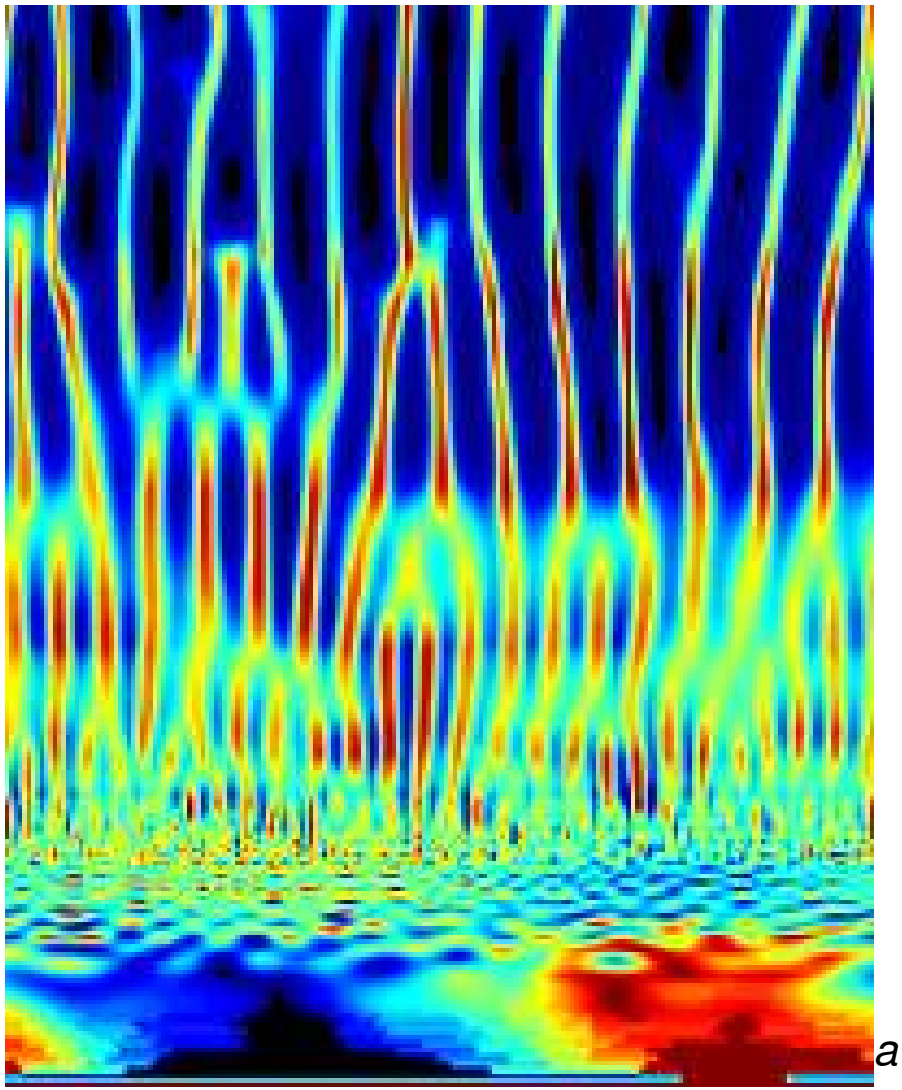
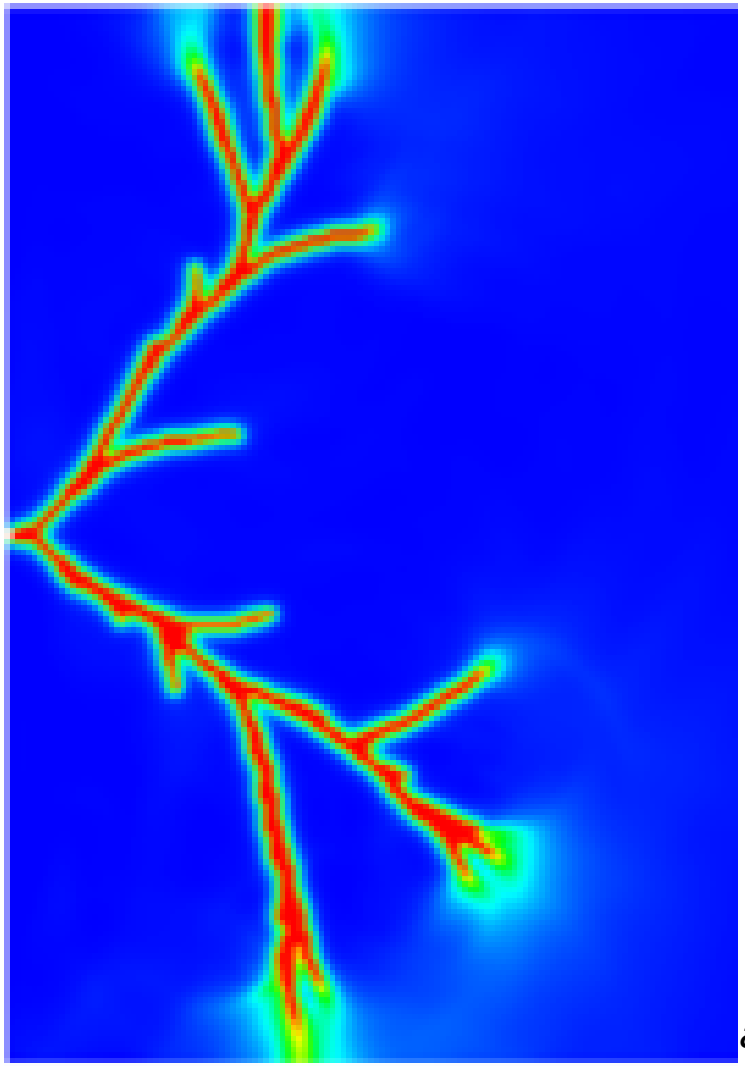


[a]Katz, Speigelman

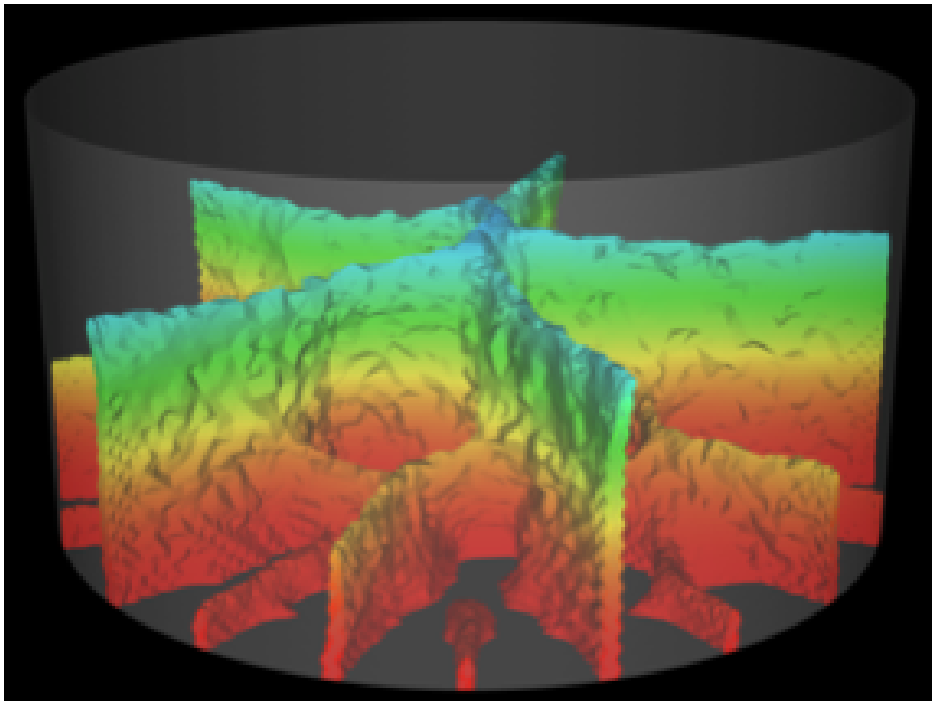
Fracture Mechanics

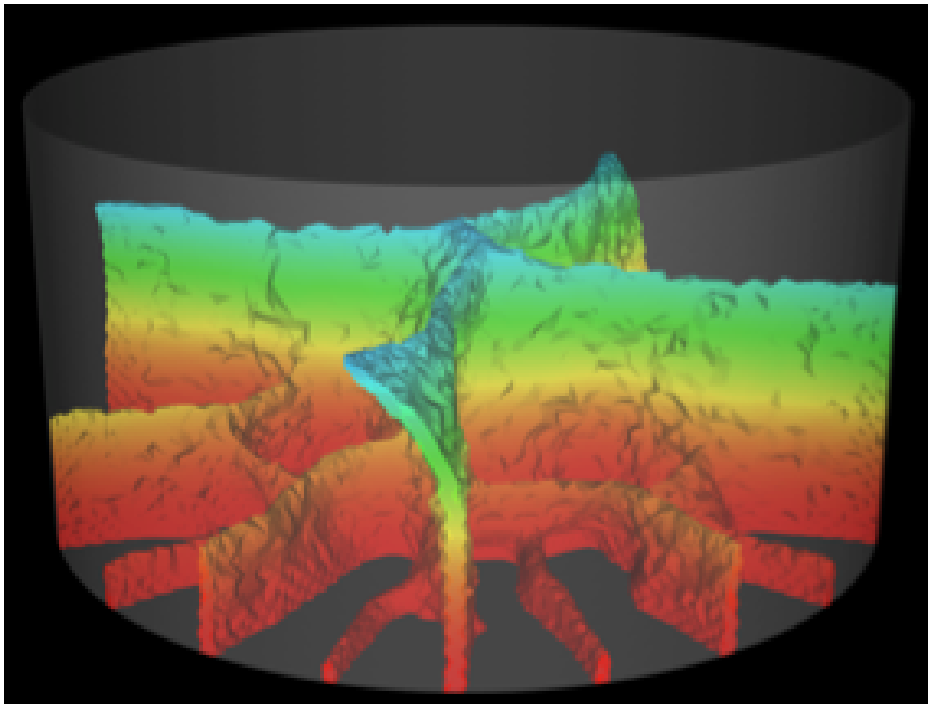
- Full variational formulation
  - Phase field
  - Linear or Quadratic penalty
- Uses TAO optimization
  - Necessary for linear penalty
  - Backtacking
- No prescribed cracks (movie)
  - Arbitrary crack geometry
  - Arbitrary intersections
- Multiple materials
  - Composite toughness



[a]Bourdin

Fracture Mechanics





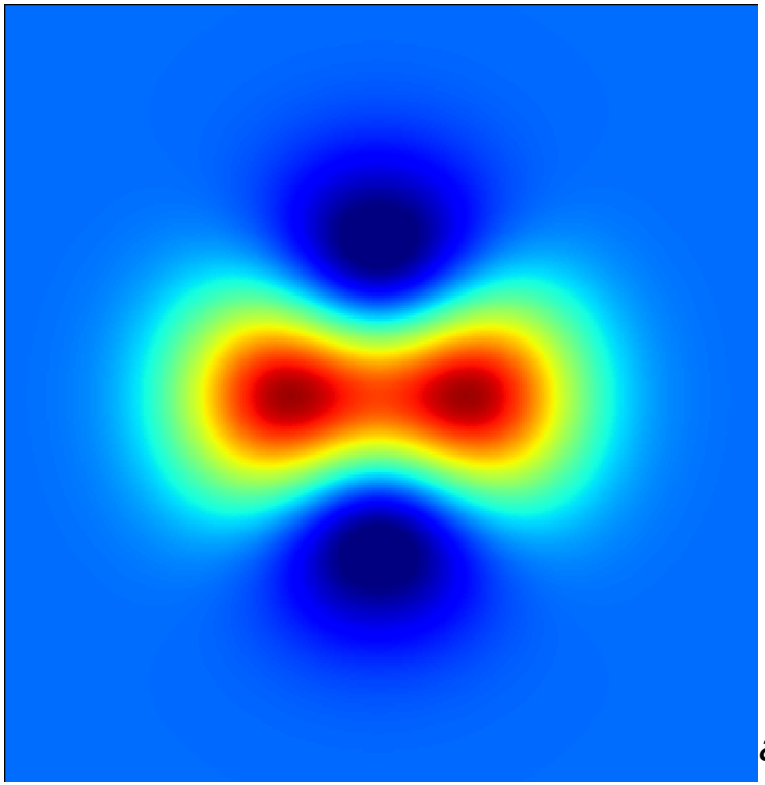
[1]

[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
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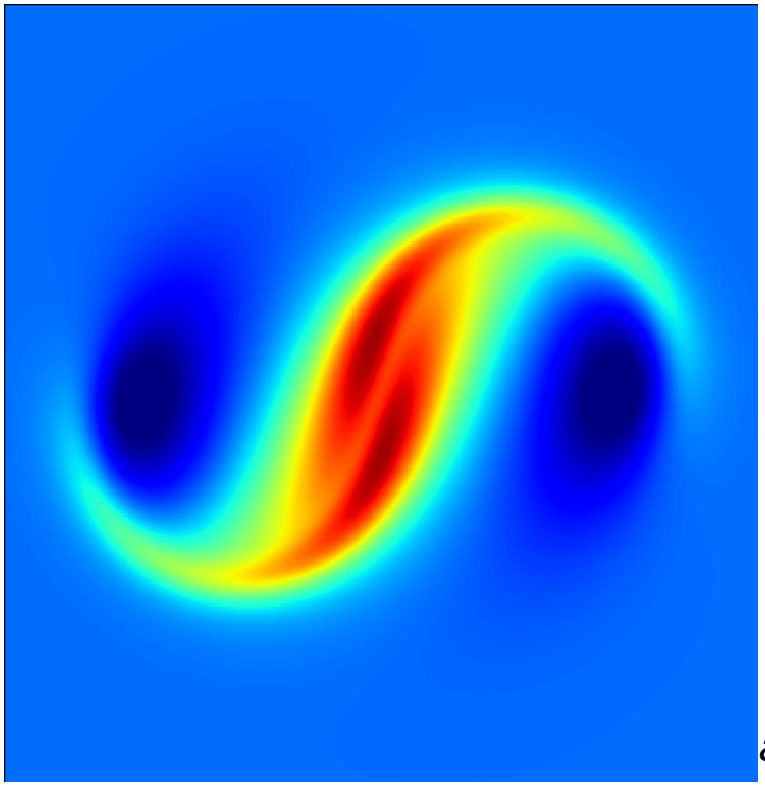

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 200

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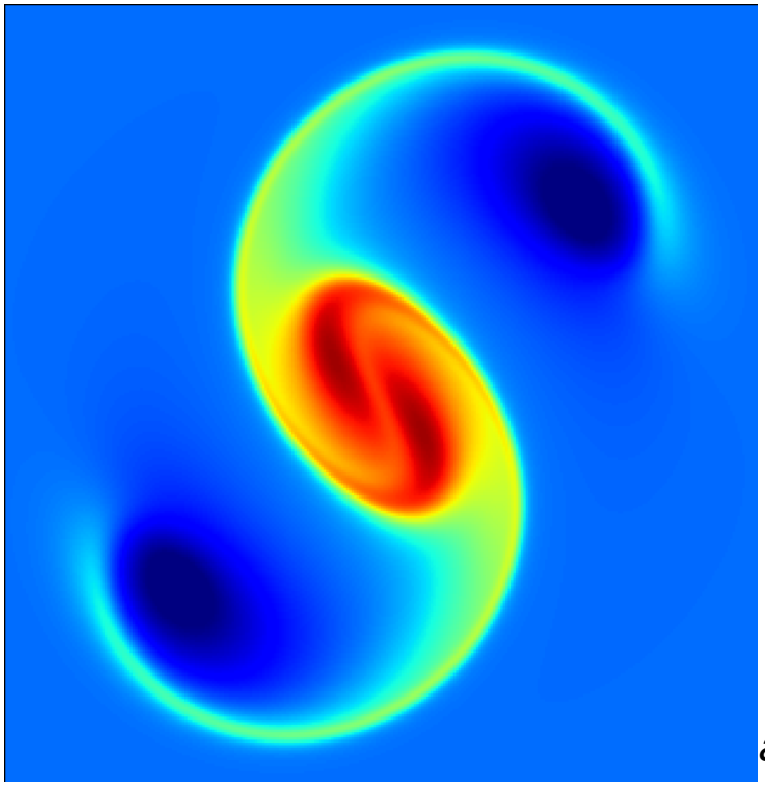

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 300

- Incompressible Flow
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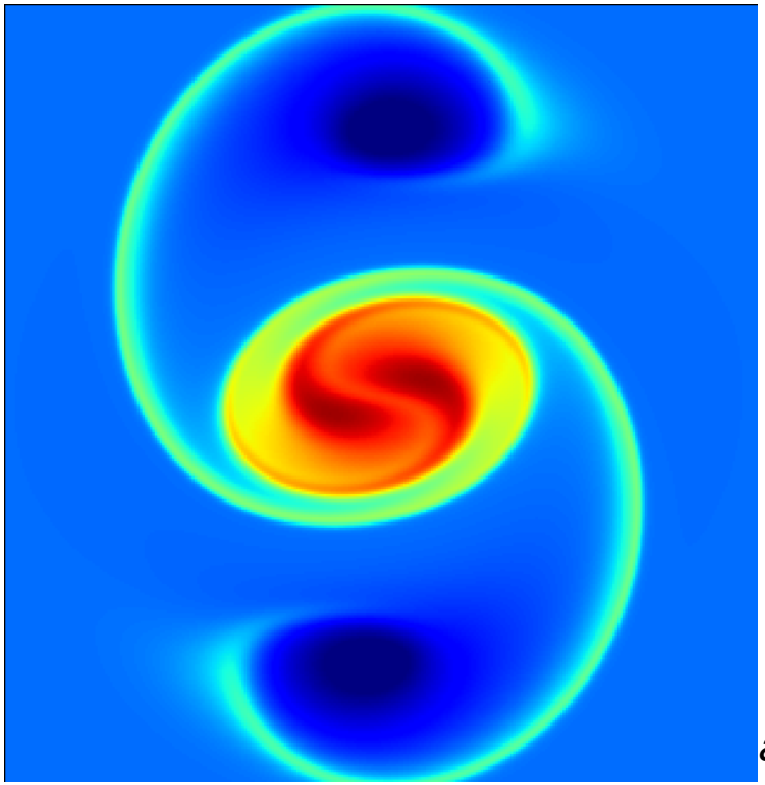

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 400

- Incompressible Flow
  - Gaussian vortex blobs
  - High Re
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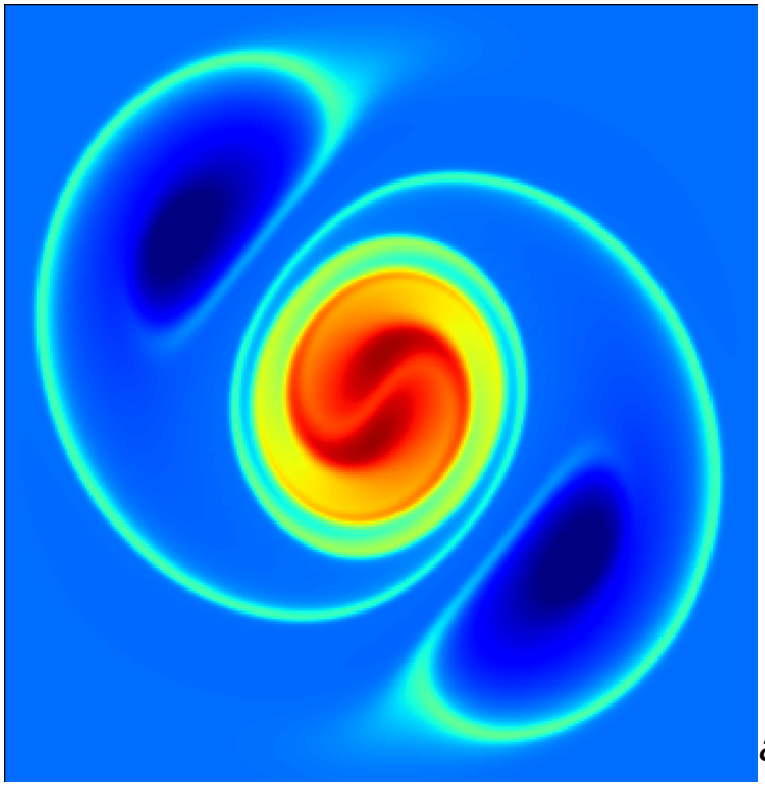

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 500

- Incompressible Flow
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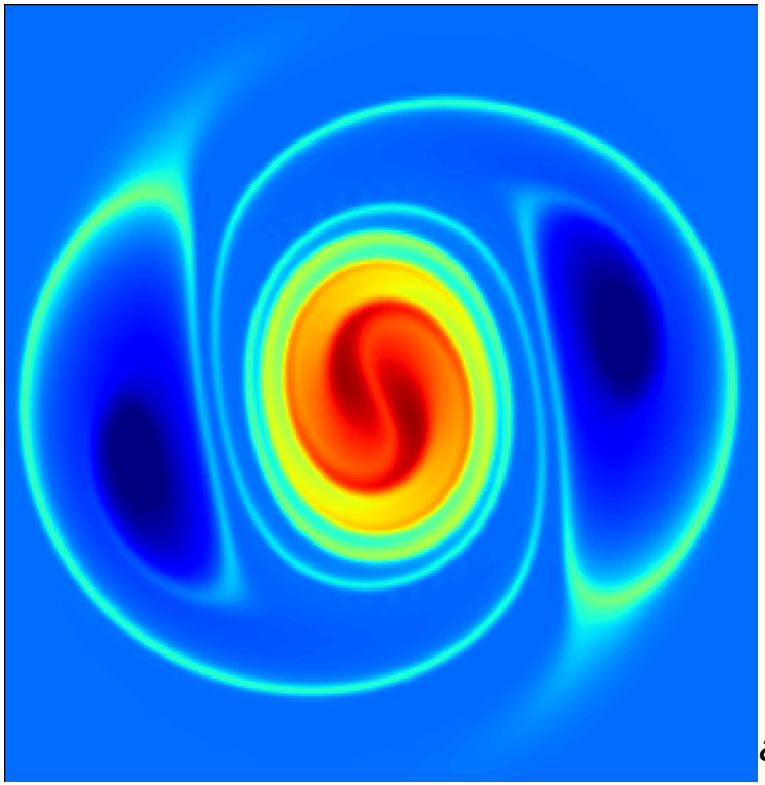

[a]Cruz, Yokota, Barba, Knepley

Vortex Method

t = 600

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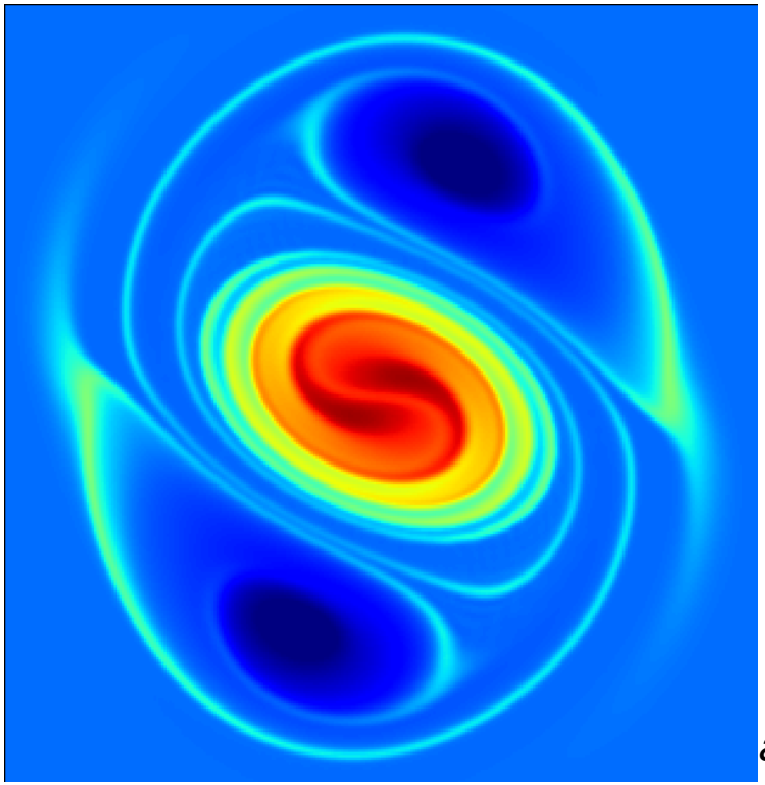

[a]Cruz, Yokota, Barba, Knepley

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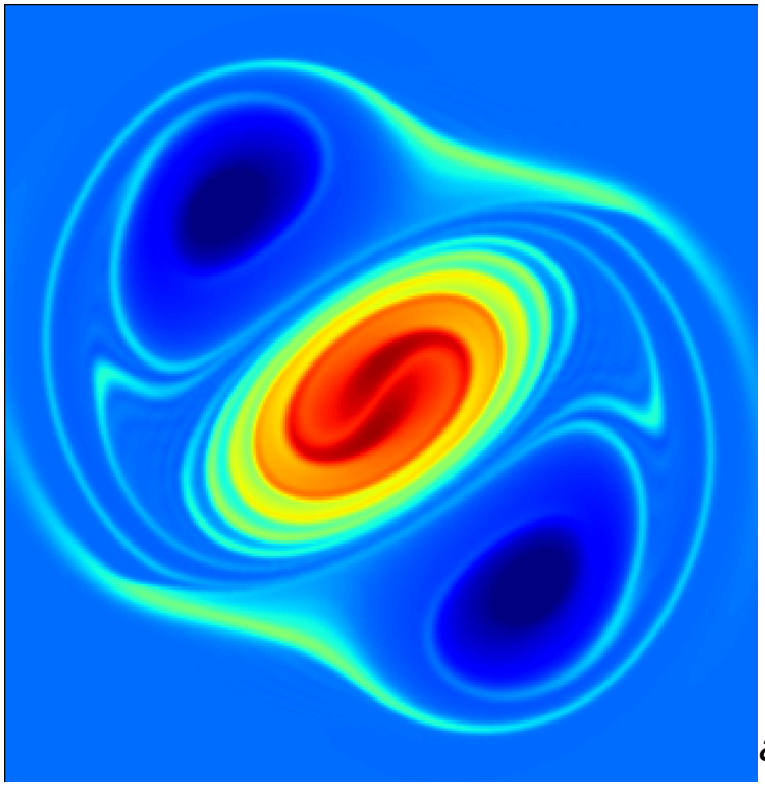

[a]Cruz, Yokota, Barba, Knepley

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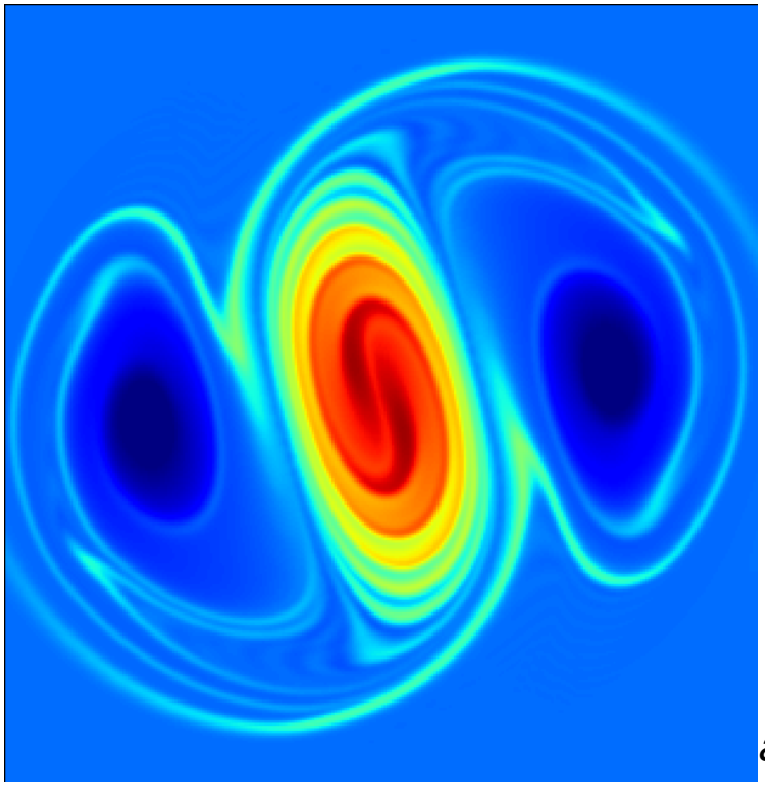
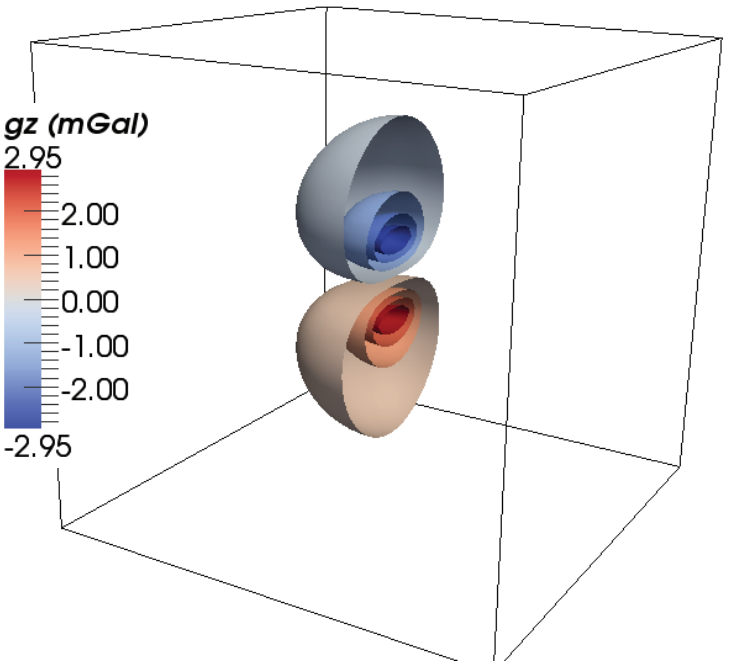


[a]Cruz, Yokota, Barba, Knepley

Gravity Anomaly Modeling

- Potential Solution
  - Kernel of inverse problem
  - Needs optimal algorithm
- Implementations
  - Direct Summation
  - FEM
  - FMM
- Parallelism
  - MPI
  - 4000+ cores
  - All methods scalable

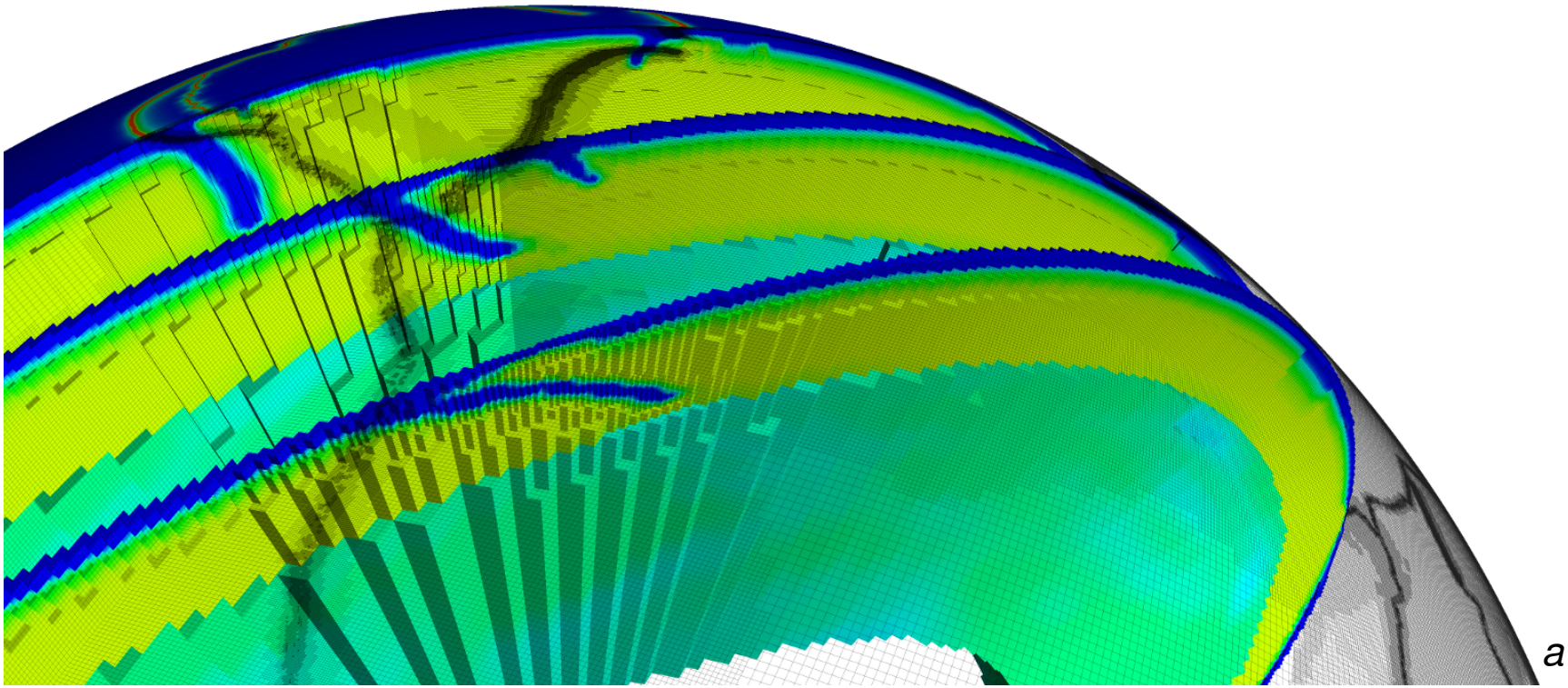


a

[a] May, Knepley

Adaptive Mesh Refinement

- DM interface with p4est package from Burstedde and Isaac
- PETSc solvers can be used seamlessly
- 2015 Gordon Bell Winner for Mantle Convection Simulation
- Inversion for basal traction on the full Antarctic ice sheet



[a]

[a] Isaac

Adaptive Mesh Refinement

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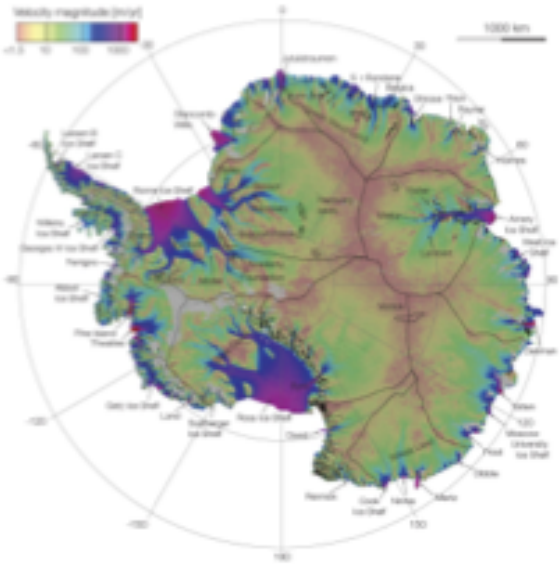
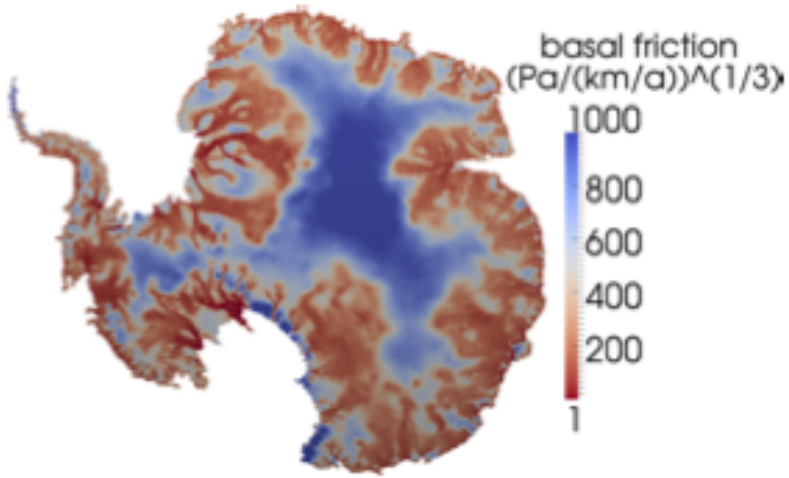


Observed surface flow velocity (Rignot et al., 2011)

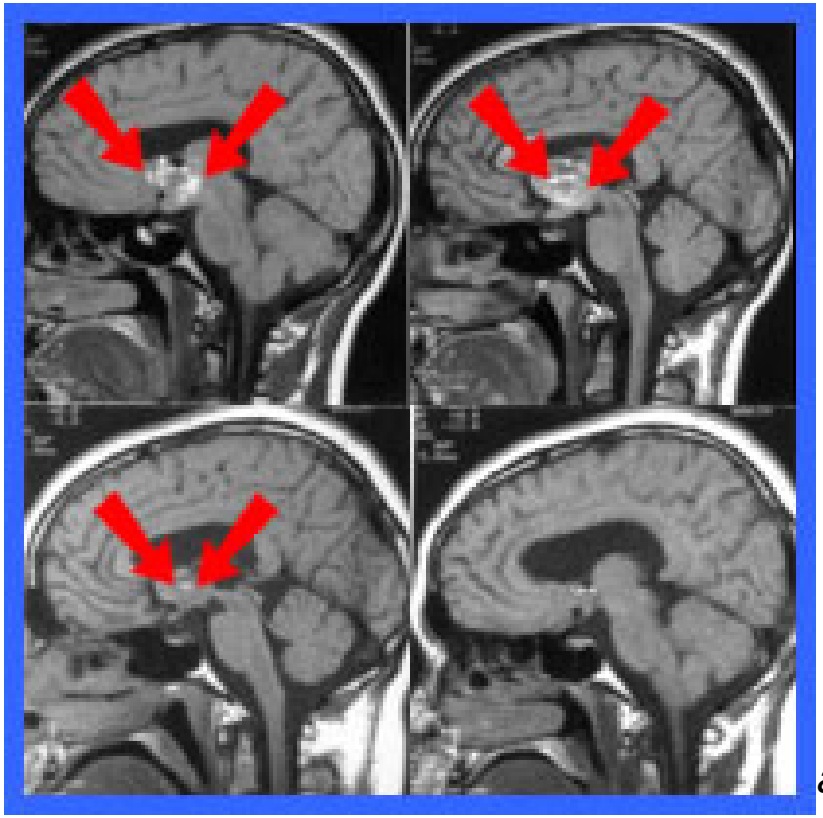


Antarctic ice sheet inversion for the basal friction parameter field using InSAR surface velocity measurements [a]

[a] Isaac

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]Warfield, Ferrant, et.al.

Real-time Surgery

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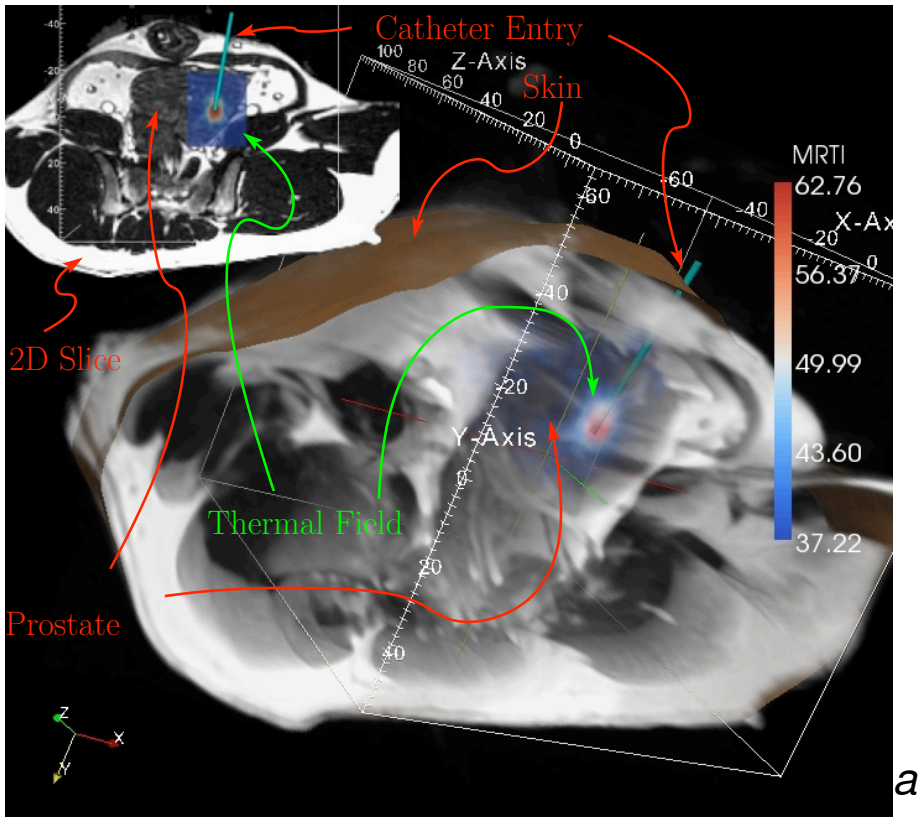

[a]

[a] Fuentes, Oden, et.al.

Outline

User Solve

```
MPI_Comm comm;
SNES snes;
DM dm;
Vec u;

SNESCreate(comm, &snes);
SNESSetDM(snes, dm);
SNESSetFromOptions(snes);
DMCreateGlobalVector(dm, &u);
SNESSolve(snes, NULL, u);
```

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), Cohouet & Chabard, IJNMF, 1988.

```
-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), Cohouet & Chabard, IJNMF, 1988.

```
-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), Elman, DTIC, 1994.

```
-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), Elman, DTIC, 1994.

```
-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, Olshanskii, et.al., Numer. Math., 2006.

```
-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, May and Moresi, PEPI, 2008.

```
-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, May and Moresi, PEPI, 2008.

```
-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 Iteration, Uzawa, 1958

```
-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, Schur, 1905.

```
-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, Patankar and Spalding, IJHMT, 1972.

```
-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, Kay, Loghin and Wathen, SISC, 2002.

```
-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, Elman, Howle, Shadid, Shuttleworth, and Tuminaro, SISC, 2006.

```
-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
```

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

Programming with Options

ex55: Allen-Cahn problem in 2D

- constant mobility
- triangular elements

Geometric multigrid method for saddle point variational inequalities:

```
./ex55 -ksp_type fgmres -pc_type mg -mg_levels_ksp_type fgmres
-mg_levels_pc_type fieldsplit -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_pc_fieldsplit_type schur -da_grid_x 65 -da_grid_y 65
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition user
-mg_levels_fieldsplit_1_ksp_type gmres -mg_coarse_ksp_type preonly
-mg_levels_fieldsplit_1_pc_type none   -mg_coarse_pc_type svd
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor    -pc_mg_levels 5
-mg_levels_fieldsplit_0_pc_sor_forward -pc_mg_galerkin
-snes_vi_monitor -ksp_monitor_true_residual -snes_atol 1.e-11
-mg_levels_ksp_monitor -mg_levels_fieldsplit_ksp_monitor
-mg_levels_ksp_max_it 2 -mg_levels_fieldsplit_ksp_max_it 5
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```
./ex55 -ksp_type fgmres -pc_type mg -pc_mg_levels 5
  -da_grid_x 65 -da_grid_y 65
```

Use the Galerkin process to compute the coarse grid operators

```
-pc_mg_galerkin
```

Use SVD as the coarse grid saddle point solver

```
-mg_coarse_ksp_type preonly -mg_coarse_pc_type svd
```

Programming with Options

ex55: Allen-Cahn problem in 2D

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```

Programming with Options

ex55: Allen-Cahn problem in 2D

Smoother: Flexible GMRES (2 iterates) with a Schur complement PC

```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```

Schur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

Programming with Options

ex55: Allen-Cahn problem in 2D

Smoother: Flexible GMRES (2 iterates) with a Schur complement PC

```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

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-mg_levels_fieldsplit_1_ksp_type gmres
-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
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```

Programming with Options

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-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

Schur complement solver: GMRES (5 iterates) with no preconditioner

```
-mg_levels_fieldsplit_1_ksp_type gmres
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```

Programming with Options

ex55: Allen-Cahn problem in 2D

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```
-mg_levels_ksp_type fgmres -mg_levels_pc_fieldsplit_detect_saddle_point
-mg_levels_ksp_max_it 2 -mg_levels_pc_type fieldsplit
-mg_levels_pc_fieldsplit_type schur
-mg_levels_pc_fieldsplit_factorization_type full
-mg_levels_pc_fieldsplit_schur_precondition diag
```

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-mg_levels_fieldsplit_1_pc_type none -mg_levels_fieldsplit_ksp_max_it 5
```
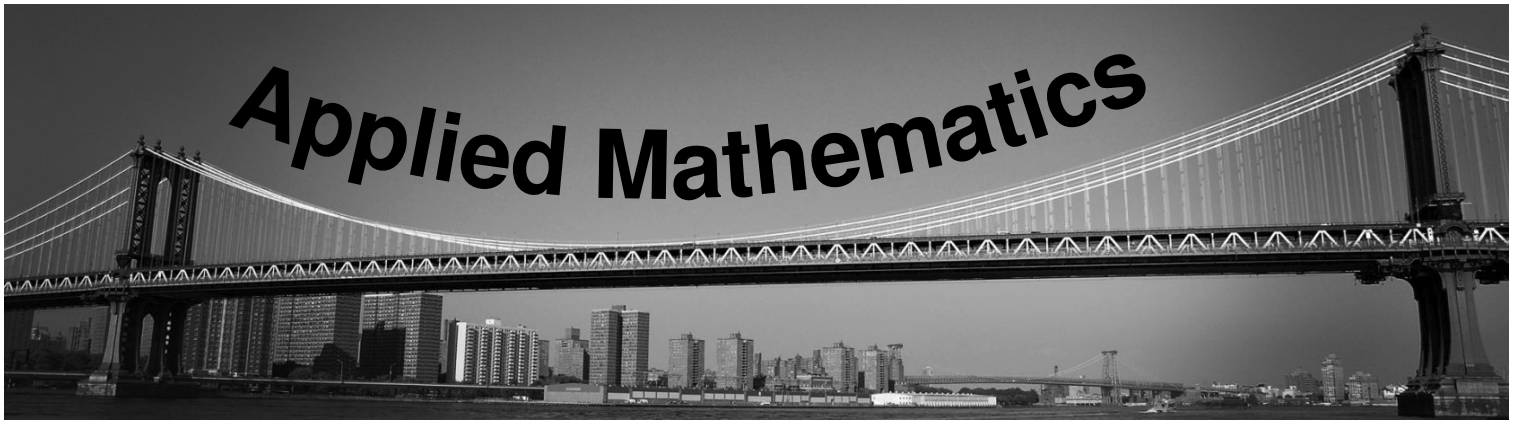

Schur complement action: Use only the lower diagonal part of A00

```
-mg_levels_fieldsplit_0_ksp_type preonly
-mg_levels_fieldsplit_0_pc_type sor
-mg_levels_fieldsplit_0_pc_sor_forward
```

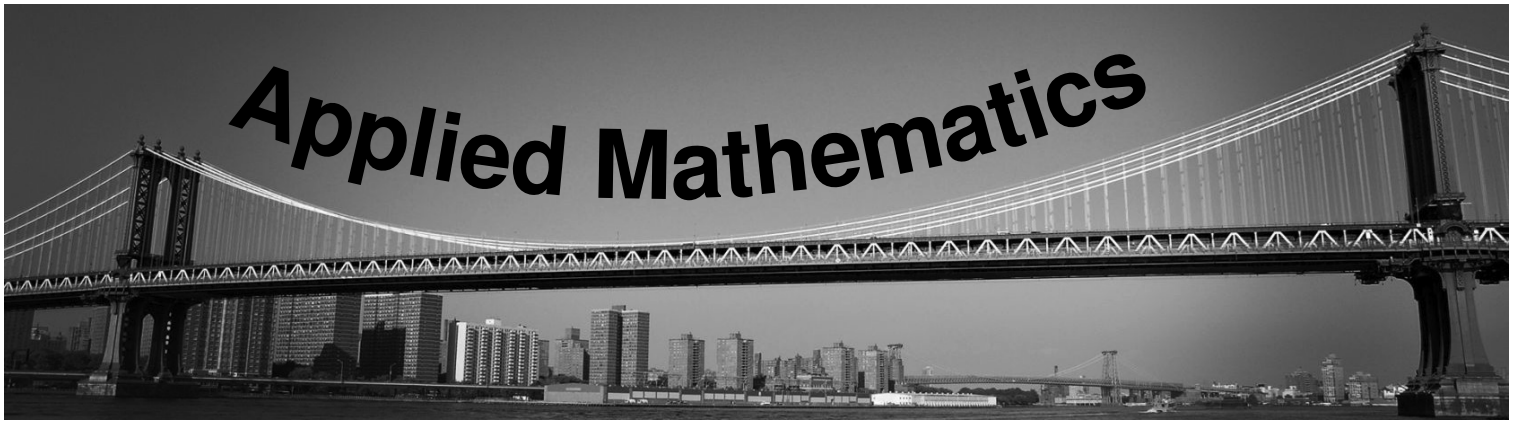
Outline

Impact of Mathematics on Science



Computational Leaders have always
embraced the latest technology
and been inspired by physical problems,

Impact of Mathematics on Science



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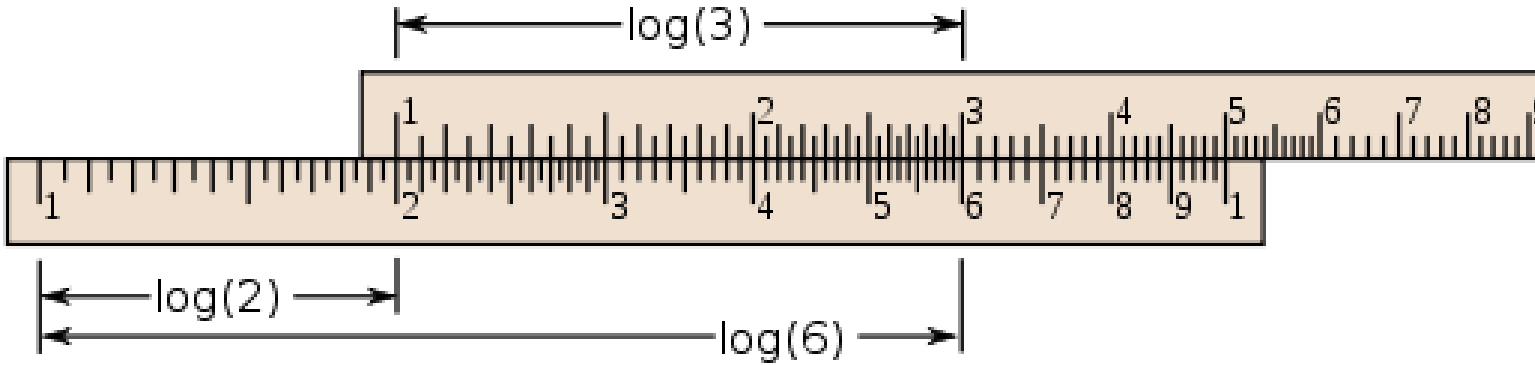
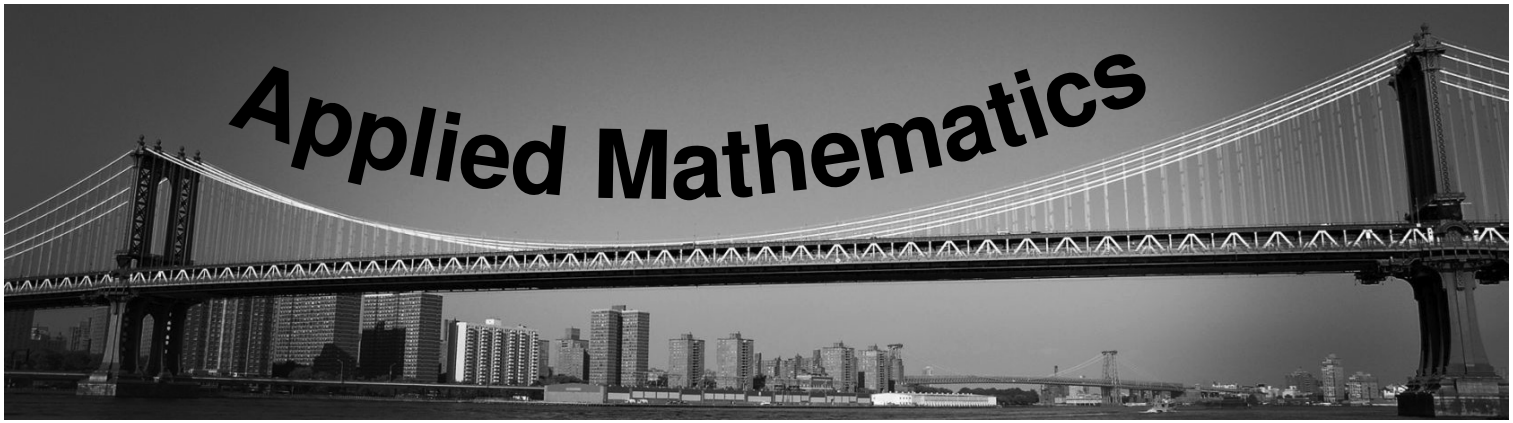


Impact of Mathematics on Science



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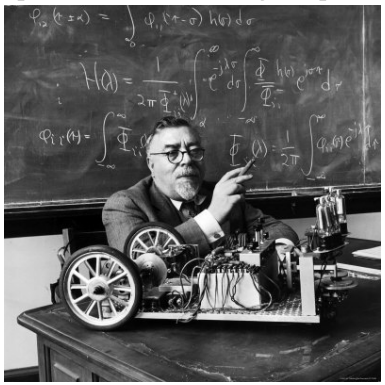
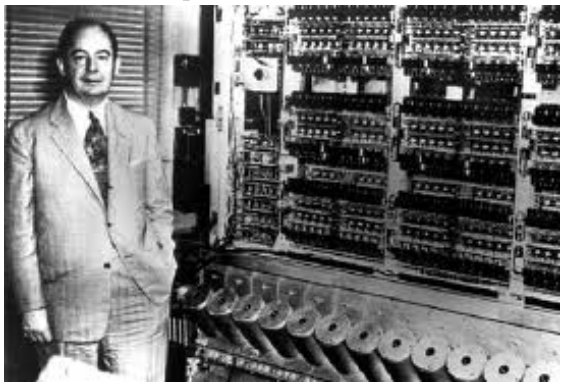
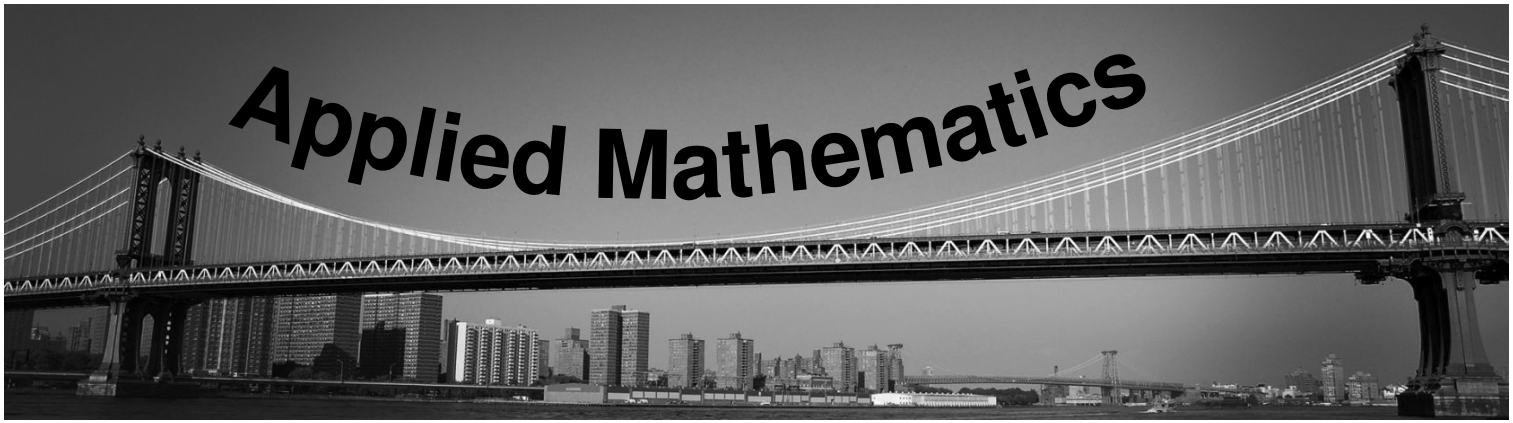




Impact of Mathematics on Science



Computational Leaders have always
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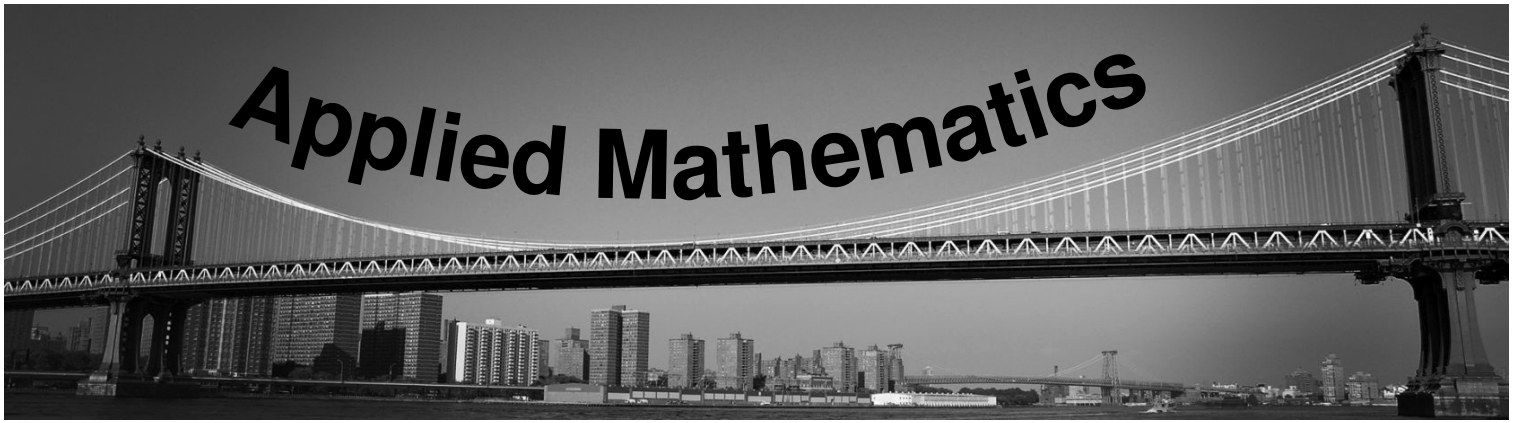
PETSc

Impact of Mathematics on Science



Computational Leaders have always
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Enabling Scientific Discovery