The Portable Extensible Toolkit for Scientific Computing

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Advanced PETSc Solvers
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Main Point

Never believe *anything*,

unless you can run it.

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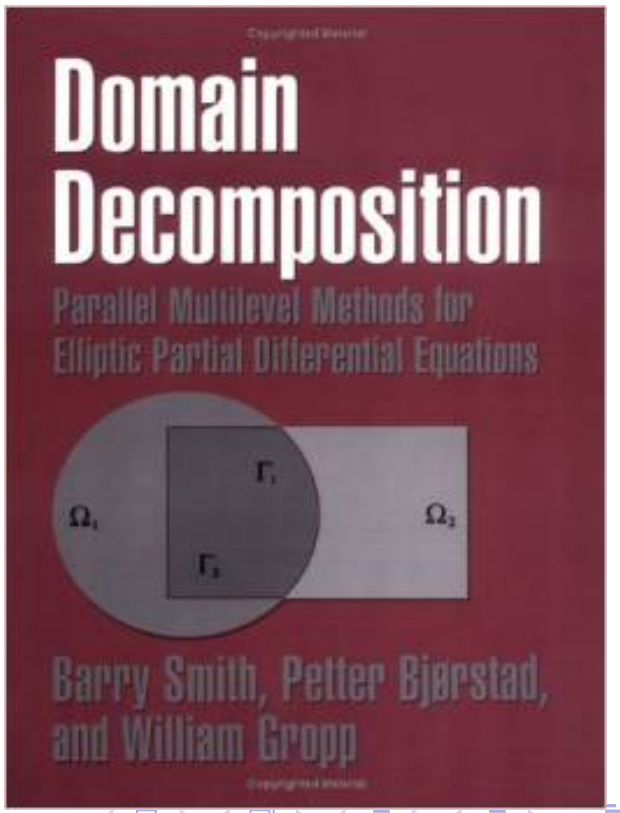
unless you can run it.

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

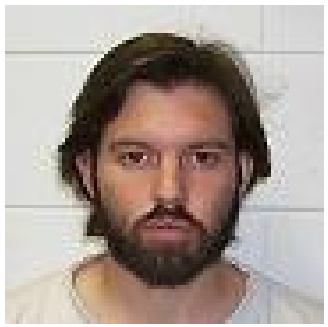
The PETSc Team


Bill Gropp


Barry Smith


Satish Balay


Jed Brown


Matt Knepley

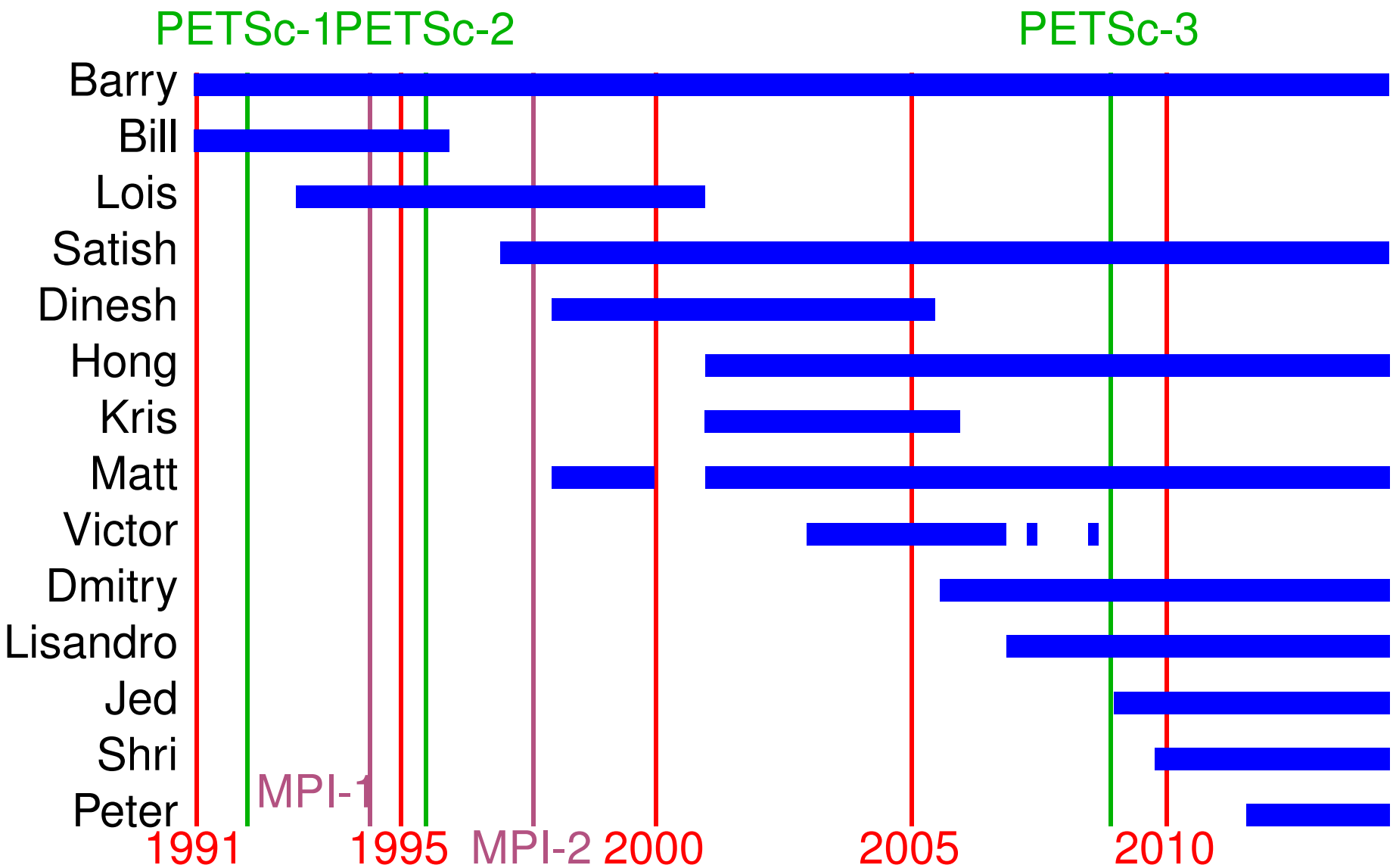

Lisandro Dalcin


Hong Zhang


Mark Adams


Toby Issac

Timeline


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

Ask Questions!!!

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

Things I Am Not Going To Talk About

- Linear Algebra (Vec/Mat)
  - TACC Tutorial
- Krylov Methods (KSP)
  - TACC Tutorial
- Preconditioners (PC)
  - TACC Tutorial
- Timestepping (TS)
  - Buffalo Tutorial
- Meshes (DMDA, DMPlex)
  - Paris Tutorial
- Data Layout (PetscSection)
  - Paris Tutorial
- Discretization (FEM/FVM)
  - Paris Tutorial

The Great Solver Schism: Monolithic or Split?

Monolithic

- Direct solvers
- Coupled Schwarz
- Coupled Neumann-Neumann (use unassembled matrices)
- Coupled Multigrid

Split

- Physics-split Schwarz (based on relaxation)
- Physics-split Schur (based on factorization)
  - SIMPLE, PCD, LSC
  - segregated smoothers
  - Augmented Lagrangian

Need to understand

- Local spectral properties
- Compatibility properties
- Global coupling strengths

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);
```

Outline

Multigrid

Multigrid is *optimal* in that is does $\mathcal{O}(N)$ work for $||r|| < \epsilon$

- Brandt, Briggs, Wan & Chan & Smith
- Constant work per level
  - Sufficiently strong solver
  - Need a constant factor decrease in the residual
- Constant factor decrease in dof
  - Log number of levels
- Sufficiently good interpolation
  - Preserves low modes
  - Cannot dump too much energy into high modes

Why Optimal Algorithms?

- The more powerful the computer,
  the greater the importance of optimality
- Example:
  - Suppose Alg_1 solves a problem in time CN^2, N is the input size
  - Suppose Alg_2 solves the same problem in time CN
  - Suppose Alg_1 and Alg_2 are able to use 10,000 processors
- In constant time compared to serial,
  - Alg1 can run a problem 100X larger
  - Alg2 can run a problem 10,000X larger
- Alternatively, filling the machine's memory,
  - Alg1 requires 100X time
  - Alg2 runs in constant time

Linear Convergence of the Poisson Problem

Convergence to $||r|| < 10^{-9}||b||$ using GMRES(30)/ILU

Elements	Iterations
128	10
256	17
512	24
1024	34
2048	67
4096	116
8192	167
16384	329
32768	558
65536	920
131072	1730

Linear Convergence of the Poisson Problem

Convergence to $||r|| < 10^{-9}||b||$ using GMRES(30)/MG

Elements	Iterations
128	5
256	7
512	6
1024	7
2048	6
4096	7
8192	6
16384	7
32768	6
65536	7
131072	6

Multigrid with DM

Allows multigrid with some simple command line options

- `-pc_type mg`, `-pc_mg_levels`
- `-pc_mg_type`, `-pc_mg_cycle_type`, `-pc_mg_galerkin`
- `-mg_levels_1_ksp_type`, `-mg_levels_1_pc_type`
- `-mg_coarse_ksp_type`, `-mg_coarse_pc_type`
- `-da_refine`, `-ksp_view`

Interface also works with GAMG and 3rd party packages like ML

A 2D Problem

Problem has:

- 1,640,961 unknowns (on the fine level)
- 8,199,681 nonzeros

	Options	Explanation
`./ex5`	`-da_grid_x 21 -da_grid_y 21`	Original grid is 21x21
	`-ksp_rtol 1.0e-9`	Solver tolerance
	`-da_refine 6`	6 levels of refinement
	`-pc_type mg`	4 levels of multigrid
	`-pc_mg_levels 4`	
	`-snes_monitor -snes_view`	Describe solver

A 3D Problem

Problem has:

- 1,689,600 unknowns (on the fine level)
- 89,395,200 nonzeros

	Options	Explanation
`./ex48`	`-M 5 -N 5`	Coarse problem size
	`-da_refine 5`	5 levels of refinement
	`-ksp_rtol 1.0e-9`	Solver tolerance
	`-thi_mat_type baij`	Needs SOR
	`-pc_type mg`	4 levels of multigrid
	`-pc_mg_levels 4`	
	`-snes_monitor -snes_view`	Describe solver

AMG

Why not use AMG?

- Of course we will try AMG
  - GAMG, `-pc_type gamg`
  - ML, `-download-ml`, `-pc_type ml`
  - BoomerAMG, `-download-hypre`, `-pc_type hypre -pc_hypre_type boomeramg`
- Problems with
  - vector character
  - anisotropy
  - scalability of setup time

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  - scalability of setup time

Outline

The Stokes Problem – Strong Form

$$
\begin{aligned}
-\Delta u + \nabla p &= f \\
\nabla \cdot u &= 0 \\
u|_{\partial\Omega} &= g \\
\int_{\Omega} p &= 0
\end{aligned}
$$

The Stokes Problem – Weak Form

For $u, v \in V$ and $p, q \in \Pi$

$$
\begin{aligned}
< \nabla v, \nabla u > - < \nabla \cdot v, p > &= < v, f > \\
< q, \nabla \cdot u > &= 0 \\
u|_{\partial\Omega} &= g \\
\int_\Omega p &= 0
\end{aligned}
$$

2D Exact Solution

$$u = x^2 + y^2$$
$$v = 2x^2 - 2xy$$
$$p = x + y - 1$$
$$f_i = 3$$

3D Exact Solution

$$u = x^2 + y^2$$
$$v = y^2 + z^2$$
$$w = x^2 + y^2 - 2(x + y)z$$
$$p = x + y + z - 3/2$$
$$f_i = 3$$

Condition of the Stokes Operator

2D P_2/P_1 Lagrange Elements

Num. Elements	Longest edge (h)	κ	L_2 error
64	1/4	7909	6.96e-07
128	$\sqrt{2}/8$	29522	1.41e-07
256	1/8	32300	7.82e-07
512	$\sqrt{2}/16$	119053	1.27e-06
256	1/16	129883	2.28e-06
1024	$\sqrt{2}/32$	466023	4.99e-06
2048	1/32	520163	6.66e-06
4096	$\sqrt{2}/64$	1121260	2.97e-05
8192	1/64	2075950	1.97e-05

so we have

$$\kappa \approx 700 h^{-2}$$

```
ex62 -interpolate -show_initial 0 -show_solution 0 -ksp_monitor
  -ksp_compute_singularvalues -pc_type none -ksp_rtol 1.0e-9
  -ksp_gmres_restart 4000 -ksp_max_it 4000 -ksp_gmres_modifiedgramschmidt
  -snes_max_linear_solve_fail 10 -refinement_limit 0.015625
```

Condition of the Stokes Operator

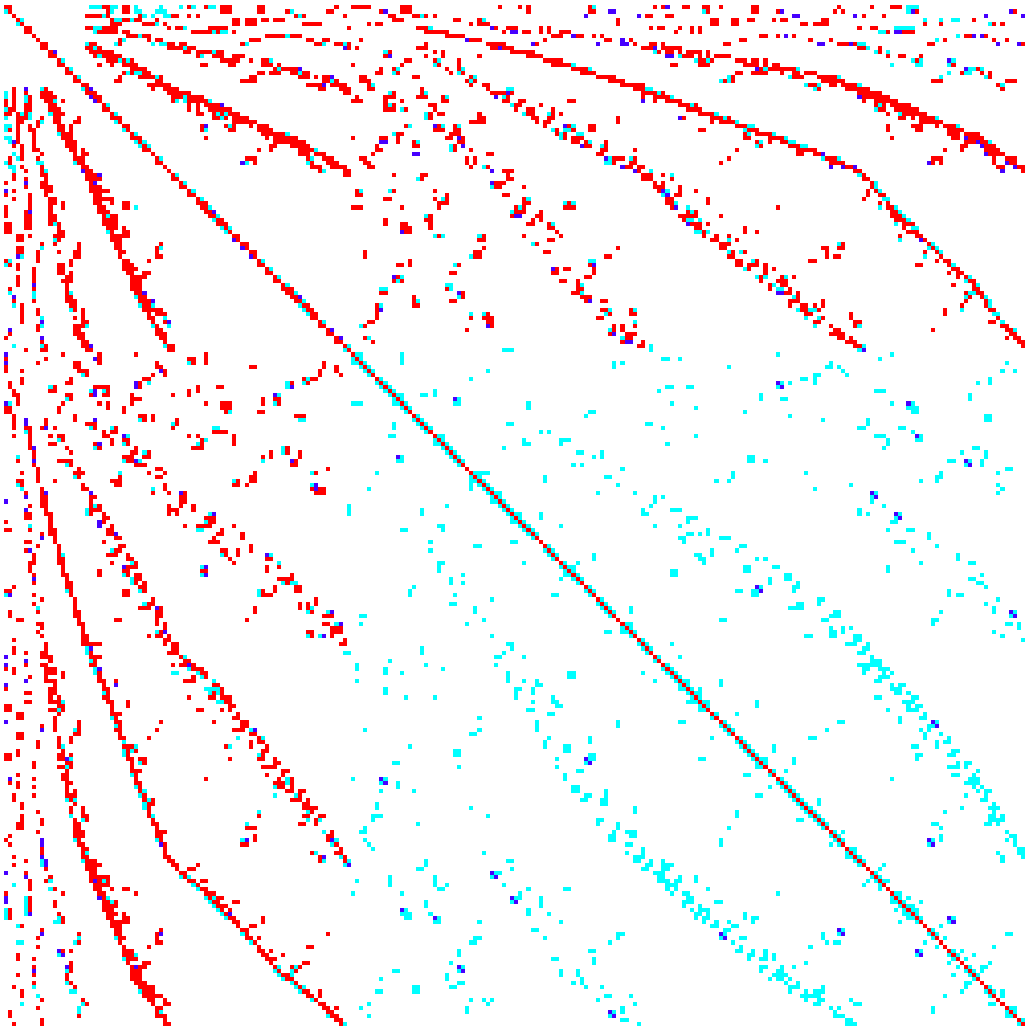
2D P_2/P_1 Lagrange Elements

```
import numpy as np
from matplotlib import pylab
from math import sqrt, exp, log

h     = np.array([1./4, sqrt(2.)/8, 1./8, sqrt(2.)/16, 1./16,
                  sqrt(2.)/32, 1./32, sqrt(2.)/64])
kappa = np.array([7909, 29522, 32300, 119053, 129883, 466023,
                  520163, 1121260])
A = np.array([-np.log(h), np.ones(len(h))])
w = np.linalg.lstsq(A.T, np.log(kappa))[0]
pylab.plot(h, kappa)
pylab.plot(h, exp(w[1])/(h*h))
pylab.show()
```

Jacobian

P_2/P_1 elements



FieldSplit Preconditioner

- Analysis
  - Use **IS**es to define fields
  - Decouples **PC** from problem definition
- Synthesis
  - Additive, Multiplicative, Schur
  - Commutes with Multigrid

FieldSplit Customization

- Analysis
  - `-pc_fieldsplit_<`**split num**`>_fields 2,1,5`
  - `-pc_fieldsplit_detect_saddle_point`
- Synthesis
  - `-pc_fieldsplit_type`
  - `-pc_fieldsplit_real_diagonal`
    Use diagonal blocks of operator to build PC
- Schur complements
  - `-pc_fieldsplit_schur_precondition <self,user,diag>`
    How to build preconditioner for S
  - `-pc_fieldsplit_schur_factorization_type <diag,lower,upper,full>`
    Which off-diagonal parts of the block factorization to use

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
```

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

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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```
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Programming with Options

ex55: Allen-Cahn problem in 2D

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Programming with Options

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

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

```
-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

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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
```

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

```
-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
```

Outline

3rd Party Solvers in PETSc

Complete table of solvers

1. Sequential LU
   - ILUDT (SPARSEKIT2, Yousef Saad, U of MN)
   - EUCLID & PILUT (Hypre, David Hysom, LLNL)
   - ESSL (IBM)
   - SuperLU (Jim Demmel and Sherry Li, LBNL)
   - Matlab
   - UMFPACK (Tim Davis, U. of Florida)
   - LUSOL (MINOS, Michael Saunders, Stanford)
2. Parallel LU
   - MUMPS (Patrick Amestoy, IRIT)
   - SPOOLES (Cleve Ashcroft, Boeing)
   - SuperLU_Dist (Jim Demmel and Sherry Li, LBNL)
3. Parallel Cholesky
   - DSCPACK (Padma Raghavan, Penn. State)
   - MUMPS (Patrick Amestoy, Toulouse)
   - CHOLMOD (Tim Davis, Florida)
4. XYTlib - parallel direct solver (Paul Fischer and Henry Tufo, ANL)

3rd Party Preconditioners in PETSc

Complete table of solvers

1. Parallel ICC
   - BlockSolve95 (Mark Jones and Paul Plassman, ANL)
2. Parallel ILU
   - PaStiX (Faverge Mathieu, INRIA)
3. Parallel Sparse Approximate Inverse
   - Parasails (Hypre, Edmund Chow, LLNL)
   - SPAI 3.0 (Marcus Grote and Barnard, NYU)
4. Sequential Algebraic Multigrid
   - RAMG (John Ruge and Klaus Steuben, GMD)
   - SAMG (Klaus Steuben, GMD)
5. Parallel Algebraic Multigrid
   - Prometheus (Mark Adams, PPPL)
   - BoomerAMG (Hypre, LLNL)
   - ML (Trilinos, Ray Tuminaro and Jonathan Hu, SNL)

Always use **SNES**

Always use **SNES** instead of **KSP**:

- No more costly than linear solver
- Can accomodate unanticipated nonlinearities
- Automatic iterative refinement
- Callback interface can take advantage of problem structure

Jed actually recommends **TS**...

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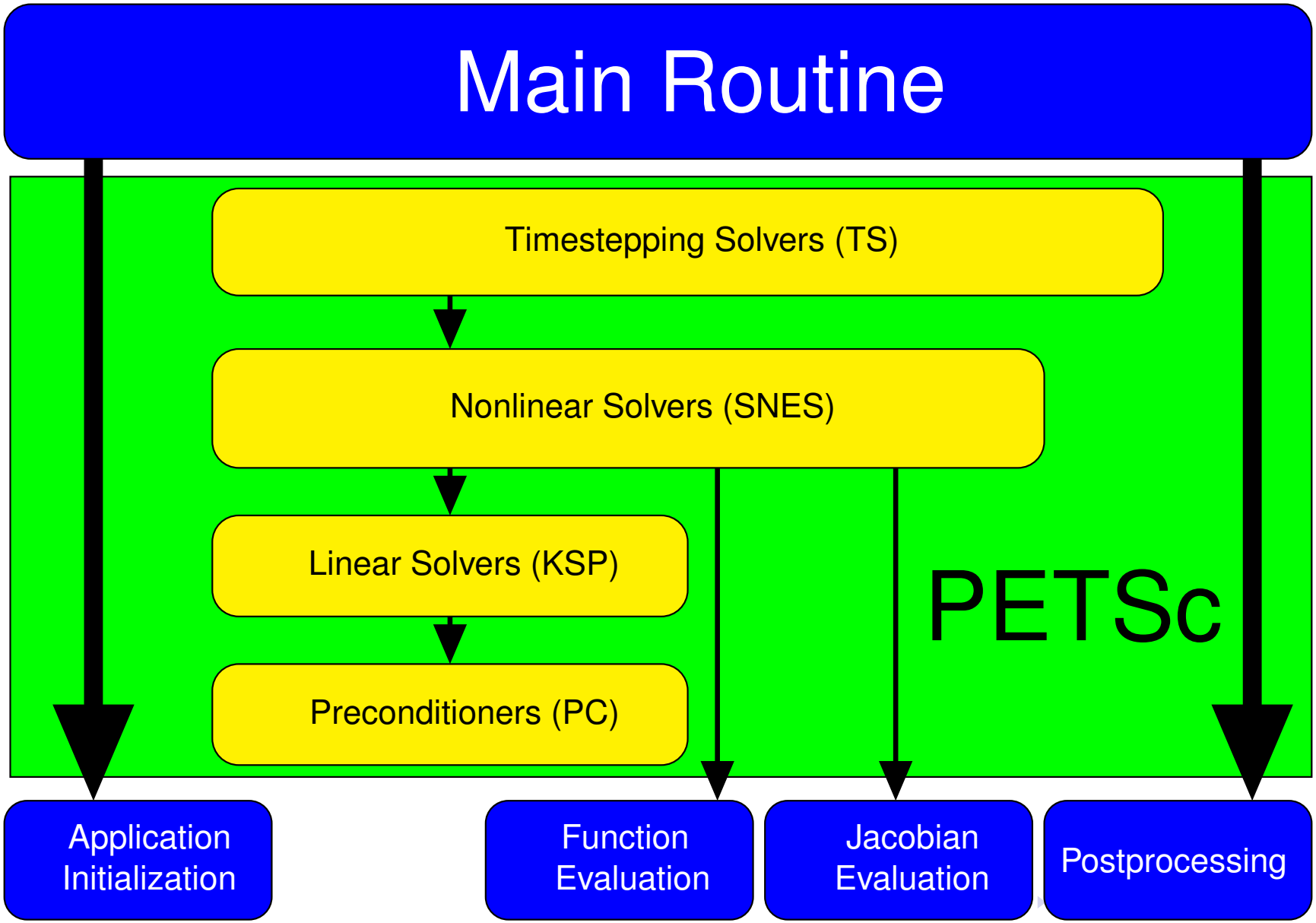
- Can accomodate unanticipated nonlinearities
- Automatic iterative refinement
- Callback interface can take advantage of problem structure

Jed actually recommends **TS**...

Flow Control for a PETSc Application



SNES Paradigm

The SNES interface is based upon callback functions

- FormFunction(), set by SNESSetFunction()
- FormJacobian(), set by SNESSetJacobian()

When PETSc needs to evaluate the nonlinear residual $F(x)$,

- Solver calls the **user's** function
- User function gets application state through the `ctx` variable
  - PETSc never sees application data

SNES Function

User provided function calculates the nonlinear residual:

```
PetscErrorCode (*func)(SNES snes,Vec x,Vec r,void *ctx)
```

- `x`: The current solution
- `r`: The residual
- `ctx`: The user context passed to SNESSetFunction()
  - Use this to pass application information, e.g. physical constants

SNES Jacobian

User provided function calculates the Jacobian:

```
PetscErrorCode (*func)(SNES snes, Vec x, Mat *J, Mat *M, void *ctx)
```

- `x`: The current solution
- `J`: The Jacobian
- `M`: The Jacobian preconditioning matrix (possibly J itself)
- `ctx`: The user context passed to SNESSetJacobian()
  - Use this to pass application information, e.g. physical constants

Alternatively, you can use

- matrix-free finite difference approximation, `-snes_mf`
- finite difference approximation with coloring, `-snes_fd`

SNES Variants

- Picard iteration
- Line search/Trust region strategies
- Quasi-Newton
- Nonlinear CG/GMRES
- Nonlinear GS/ASM
- Nonlinear Multigrid (FAS)
- Variational inequality approaches

New methods in SNES

LS, TR	Newton-type with line search and trust region
NRichardson	Nonlinear Richardson, usually preconditioned
VIRS, VISS	reduced space and semi-smooth methods for variational inequalities
QN	Quasi-Newton methods like BFGS
NGMRES	Nonlinear GMRES
NCG	Nonlinear Conjugate Gradients
SORQN	SOR quasi-Newton
GS	Nonlinear Gauss-Seidel sweeps
FAS	Full approximation scheme (nonlinear multigrid)
MS	Multi-stage smoothers (in FAS for hyperbolic problems)
Shell	Your method, often used as a (nonlinear) preconditioner

Finite Difference Jacobians

PETSc can compute and explicitly store a Jacobian via 1st-order FD

- Dense
  - Activated by `-snes_fd`
  - Computed by SNESDefaultComputeJacobian()
- Sparse via colorings (default)
  - Coloring is created by MatFDColoringCreate()
  - Computed by SNESDefaultComputeJacobianColor()

Can also use Matrix-free Newton-Krylov via 1st-order FD

- Activated by `-snes_mf` without preconditioning
- Activated by `-snes_mf_operator` with user-defined preconditioning
  - Uses preconditioning matrix from SNESSetJacobian()

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e2
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e2
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view

lid velocity = 100, prandtl # = 1, grashof # = 100
  0 SNES Function norm 768.116
  1 SNES Function norm 658.288
  2 SNES Function norm 529.404
  3 SNES Function norm 377.51
  4 SNES Function norm 304.723
  5 SNES Function norm 2.59998
  6 SNES Function norm 0.00942733
  7 SNES Function norm 5.20667e-08
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 7
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view

lid velocity = 100, prandtl # = 1, grashof # = 10000
  0 SNES Function norm 785.404
  1 SNES Function norm 663.055
  2 SNES Function norm 519.583
  3 SNES Function norm 360.87
  4 SNES Function norm 245.893
  5 SNES Function norm 1.8117
  6 SNES Function norm 0.00468828
  7 SNES Function norm 4.417e-08
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 7
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e5
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e5
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_monitor_short -snes_converged_reason -snes_view

lid velocity = 100, prandtl # = 1, grashof # = 100000
  0 SNES Function norm 1809.96
Nonlinear solve did not converge due to DIVERGED_LINEAR_SOLVE iterations 0
```

Driven Cavity Problem

SNES ex19.c

```
./ex19 -lidvelocity 100 -grashof 1e5
  -da_grid_x 16 -da_grid_y 16 -da_refine 2 -pc_type lu
  -snes_monitor_short -snes_converged_reason -snes_view

lid velocity = 100, prandtl # = 1, grashof # = 100000
  0 SNES Function norm 1809.96
  1 SNES Function norm 1678.37
  2 SNES Function norm 1643.76
  3 SNES Function norm 1559.34
  4 SNES Function norm 1557.6
  5 SNES Function norm 1510.71
  6 SNES Function norm 1500.47
  7 SNES Function norm 1498.93
  8 SNES Function norm 1498.44
  9 SNES Function norm 1498.27
 10 SNES Function norm 1498.18
 11 SNES Function norm 1498.12
 12 SNES Function norm 1498.11
 13 SNES Function norm 1498.11
 14 SNES Function norm 1498.11
 ...
```

Why isn't SNES converging?

- The Jacobian is wrong (maybe only in parallel)
  - Check with `-snes_type test` and `-snes_mf_operator -pc_type lu`
- The linear system is not solved accurately enough
  - Check with `-pc_type lu`
  - Check `-ksp_monitor_true_residual`, try right preconditioning
- The Jacobian is singular with inconsistent right side
  - Use **MatNullSpace** to inform the **KSP** of a known null space
  - Use a different Krylov method or preconditioner
- The nonlinearity is just really strong
  - Run with `-info` or `-snes_ls_monitor` to see line search
  - Try using trust region instead of line search `-snes_type tr`
  - Try grid sequencing if possible `-snes_grid_sequence`
  - Use a continuation

Nonlinear Preconditioning

PC preconditions **KSP**

```
-ksp_type gmres
```

```
-pc_type richardson
```

SNES preconditions **SNES**

```
-snes_type ngmres
```

```
-npc_snes_type nrichardson
```

Nonlinear Preconditioning

PC preconditions **KSP**

```
-ksp_type gmres

-pc_type richardson
```

SNES preconditions **SNES**

```
-snes_type ngmres

-npc_snes_type nrichardson
```

Nonlinear Use Cases

Warm start Newton

```
-snes_type newtonls
-npc_snes_type nrichardson -npc_snes_max_it 5
```

Cleanup noisy Jacobian

```
-snes_type ngmres -snes_ngmres_m 5
-npc_snes_type newtonls
```

Additive-Schwarz Preconditioned Inexact Newton

```
-snes_type aspin -snes_npc_side left
-npc_snes_type nasm -npc_snes_nasm_type restrict
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type newtonls -snes_converged_reason
 -pc_type lu
```

```
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
  1 SNES Function norm 1132.29
  2 SNES Function norm 1026.17
  3 SNES Function norm 925.717
  4 SNES Function norm 924.778
  5 SNES Function norm 836.867
  :
 21 SNES Function norm 585.143
 22 SNES Function norm 585.142
 23 SNES Function norm 585.142
 24 SNES Function norm 585.142
  :
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type fas -snes_converged_reason
 -fas_levels_snes_type gs -fas_levels_snes_max_it 6
```

```
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
  1 SNES Function norm 574.793
  2 SNES Function norm 513.02
  3 SNES Function norm 216.721
  4 SNES Function norm 85.949
Nonlinear solve did not converge due to DIVERGED_INNER iterations 4
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type fas -snes_converged_reason
 -fas_levels_snes_type gs -fas_levels_snes_max_it 6
  -fas_coarse_snes_converged_reason
```

```
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 12
  1 SNES Function norm 574.793
    Nonlinear solve did not converge due to DIVERGED_MAX_IT its 50
  2 SNES Function norm 513.02
    Nonlinear solve did not converge due to DIVERGED_MAX_IT its 50
  3 SNES Function norm 216.721
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 22
  4 SNES Function norm 85.949
    Nonlinear solve did not converge due to DIVERGED_LINE_SEARCH its 42
Nonlinear solve did not converge due to DIVERGED_INNER iterations 4
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type fas -snes_converged_reason
 -fas_levels_snes_type gs -fas_levels_snes_max_it 6
  -fas_coarse_snes_linesearch_type basic
  -fas_coarse_snes_converged_reason


lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 6
  :
 47 SNES Function norm 78.8401
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 5
 48 SNES Function norm 73.1185
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 6
 49 SNES Function norm 78.834
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 5
 50 SNES Function norm 73.1176
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 6
  :
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type nrichardson -npc_snes_max_it 1 -snes_converged_reason
 -npc_snes_type fas -npc_fas_coarse_snes_converged_reason
  -npc_fas_levels_snes_type gs -npc_fas_levels_snes_max_it 6
  -npc_fas_coarse_snes_linesearch_type basic
```

```
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 6
  1 SNES Function norm 552.271
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 27
  2 SNES Function norm 173.45
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 45
  ⋮
 43 SNES Function norm 3.45407e-05
    Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
 44 SNES Function norm 1.6141e-05
    Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
 45 SNES Function norm 9.13386e-06
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 45
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type ngmres -npc_snes_max_it 1 -snes_converged_reason
 -npc_snes_type fas -npc_fas_coarse_snes_converged_reason
  -npc_fas_levels_snes_type gs -npc_fas_levels_snes_max_it 6
  -npc_fas_coarse_snes_linesearch_type basic
```

```
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 6
  1 SNES Function norm 538.605
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 13
  2 SNES Function norm 178.005
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 24
  ⋮
 27 SNES Function norm 0.000102487
    Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 2
 28 SNES Function norm 4.2744e-05
    Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
 29 SNES Function norm 1.01621e-05
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 29
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type ngmres -npc_snes_max_it 1 -snes_converged_reason
 -npc_snes_type fas -npc_fas_coarse_snes_converged_reason
 -npc_fas_levels_snes_type newtonls -npc_fas_levels_snes_max_it 6
  -npc_fas_levels_snes_linesearch_type basic
  -npc_fas_levels_snes_max_linear_solve_fail 30
  -npc_fas_levels_ksp_max_it 20 -npc_fas_levels_snes_converged_reason
  -npc_fas_coarse_snes_linesearch_type basic
lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
    Nonlinear solve did not converge due to DIVERGED_MAX_IT its 6
    :
    :
        Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 1
    :
    :
  1 SNES Function norm 0.1935
  2 SNES Function norm 0.0179938
  3 SNES Function norm 0.00223698
  4 SNES Function norm 0.000190461
  5 SNES Function norm 1.6946e-06
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 5
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type composite -snes_composite_type additiveoptimal
 -snes_composite_sneses fas,newtonls -snes_converged_reason
 -sub_0_fas_levels_snes_type gs -sub_0_fas_levels_snes_max_it 6
   -sub_0_fas_coarse_snes_linesearch_type basic
 -sub_1_snes_linesearch_type basic -sub_1_pc_type mg


lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
  1 SNES Function norm 541.462
  2 SNES Function norm 162.92
  3 SNES Function norm 48.8138
  4 SNES Function norm 11.1822
  5 SNES Function norm 0.181469
  6 SNES Function norm 0.00170909
  7 SNES Function norm 3.24991e-08
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 7
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type composite -snes_composite_type multiplicative
 -snes_composite_sneses fas,newtonls -snes_converged_reason
 -sub_0_fas_levels_snes_type gs -sub_0_fas_levels_snes_max_it 6
   -sub_0_fas_coarse_snes_linesearch_type basic
 -sub_1_snes_linesearch_type basic -sub_1_pc_type mg


lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
  1 SNES Function norm 544.404
  2 SNES Function norm 18.2513
  3 SNES Function norm 0.488689
  4 SNES Function norm 0.000108712
  5 SNES Function norm 5.68497e-08
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 5
```

Nonlinear Preconditioning

Solver	T	N. It	L. It	Func	Jac	PC	NPC
$(\mathcal{N}\backslash \mathrm{K}-\mathrm{MG})$	9.83	17	352	34	85	370	–
NGMRES $-_R$ $(\mathcal{N}\backslash \mathrm{K}-\mathrm{MG})$	7.48	10	220	21	50	231	10
FAS	6.23	162	0	2382	377	754	–
FAS $+$ $(\mathcal{N}\backslash \mathrm{K}-\mathrm{MG})$	8.07	10	197	232	90	288	–
FAS $*$ $(\mathcal{N}\backslash \mathrm{K}-\mathrm{MG})$	4.01	5	80	103	45	125	–
NRICH $-_L$ FAS	3.20	50	0	1180	192	384	50
NGMRES $-_R$ FAS	1.91	24	0	447	83	166	24

Nonlinear Preconditioning

See discussion in:

Composing scalable nonlinear solvers,
Peter Brune, Matthew Knepley, Barry Smith, and Xuemin Tu,

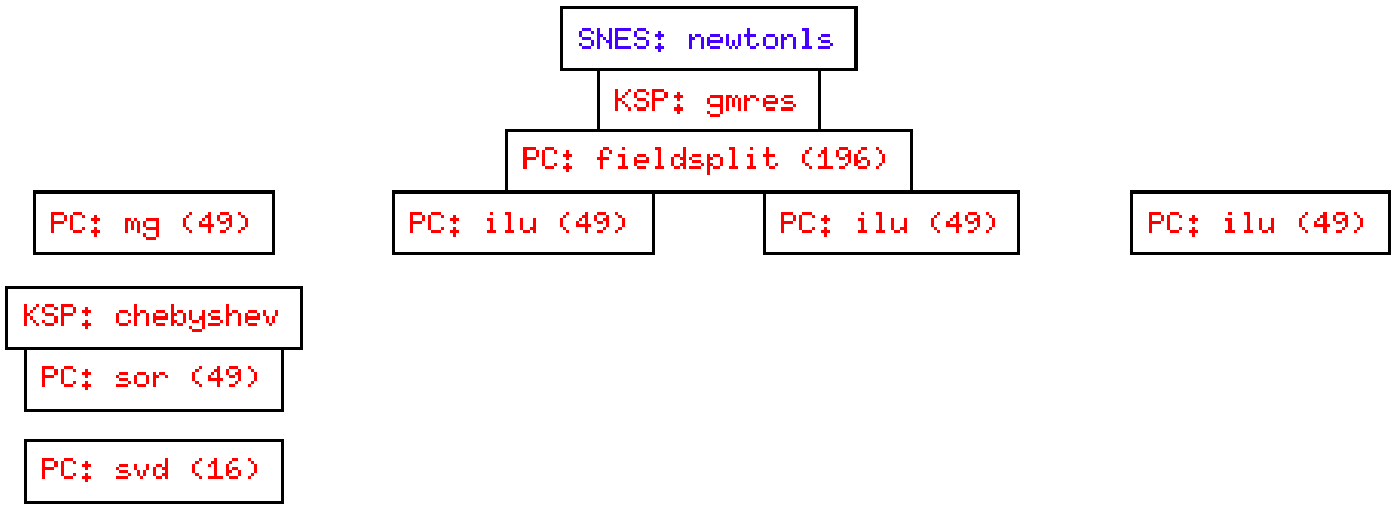
ANL/MCS-P2010-0112, Argonne National Laboratory, 2012.

http://www.mcs.anl.gov/uploads/cels/papers/P2010-0112.pdf

Visualizing Solvers

This shows how to visualize a nested solver configuration:

```
./ex19 -da_refine 1 -pc_type fieldsplit -fieldsplit_x_velocity_pc_type mg
  -fieldsplit_x_velocity_mg_coarse_pc_type svd
  -snes_view draw -draw_pause -2 -geometry 0,0,600,600
```



Conclusions

PETSc can help you:

- easily construct a code to test your ideas
  - Lots of code construction, management, and debugging tools
- scale an existing code to large or distributed machines
  - Using `FormFunctionLocal()` and scalable linear algebra
- incorporate more scalable or higher performance algorithms
  - Such as domain decomposition, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations

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Conclusions

PETSc can help you:

- easily construct a code to test your ideas
  - Lots of code construction, management, and debugging tools
- scale an existing code to large or distributed machines
  - Using `FormFunctionLocal()` and scalable linear algebra
- incorporate more scalable or higher performance algorithms
  - Such as domain decomposition, fieldsplit, and multigrid
- tune your code to new architectures
  - Using profiling tools and specialized implementations