An Introduction to PETSc

Matthew Knepley

Computer Science and Engineering
University at Buffalo

SIAM Geosciences
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Outline

Libraries Hide Hardware Details

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Why Libraries?

Libraries Hide Hardware Details

Libraries Hide Implementation Complexity

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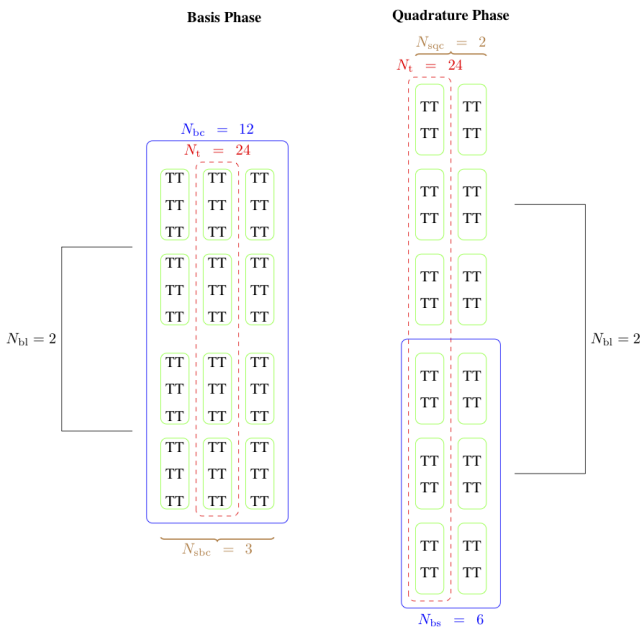

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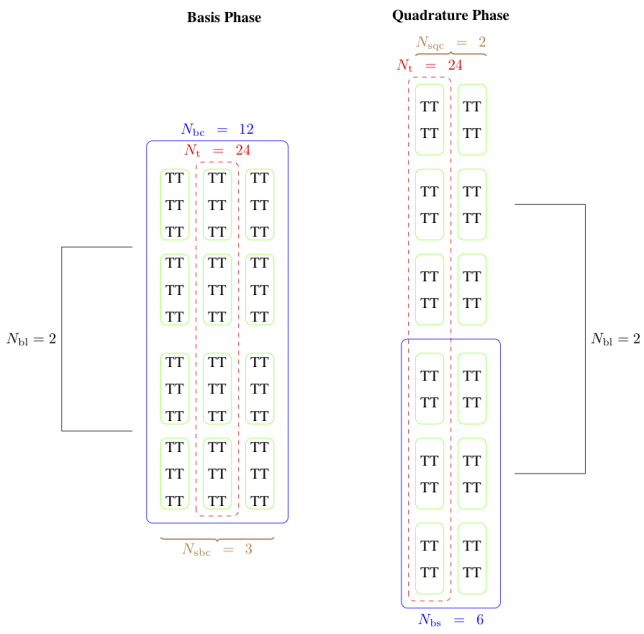

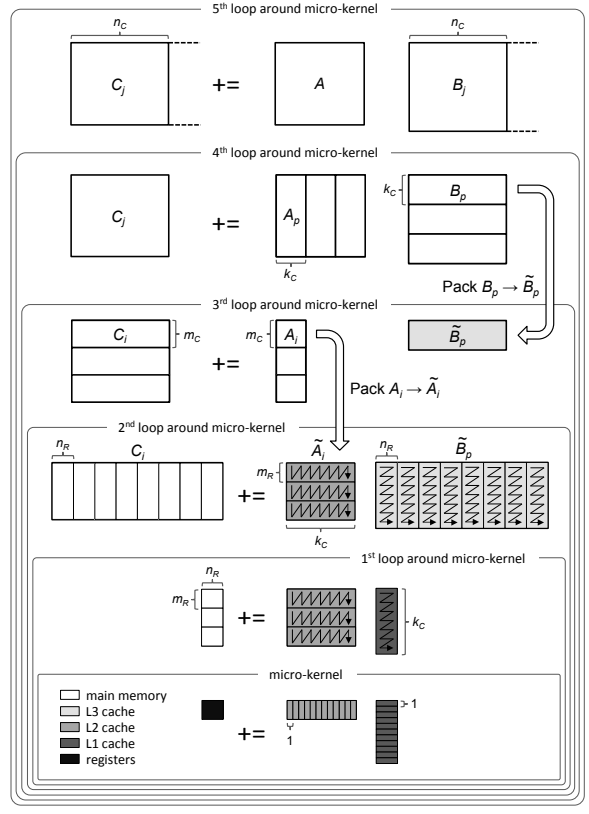

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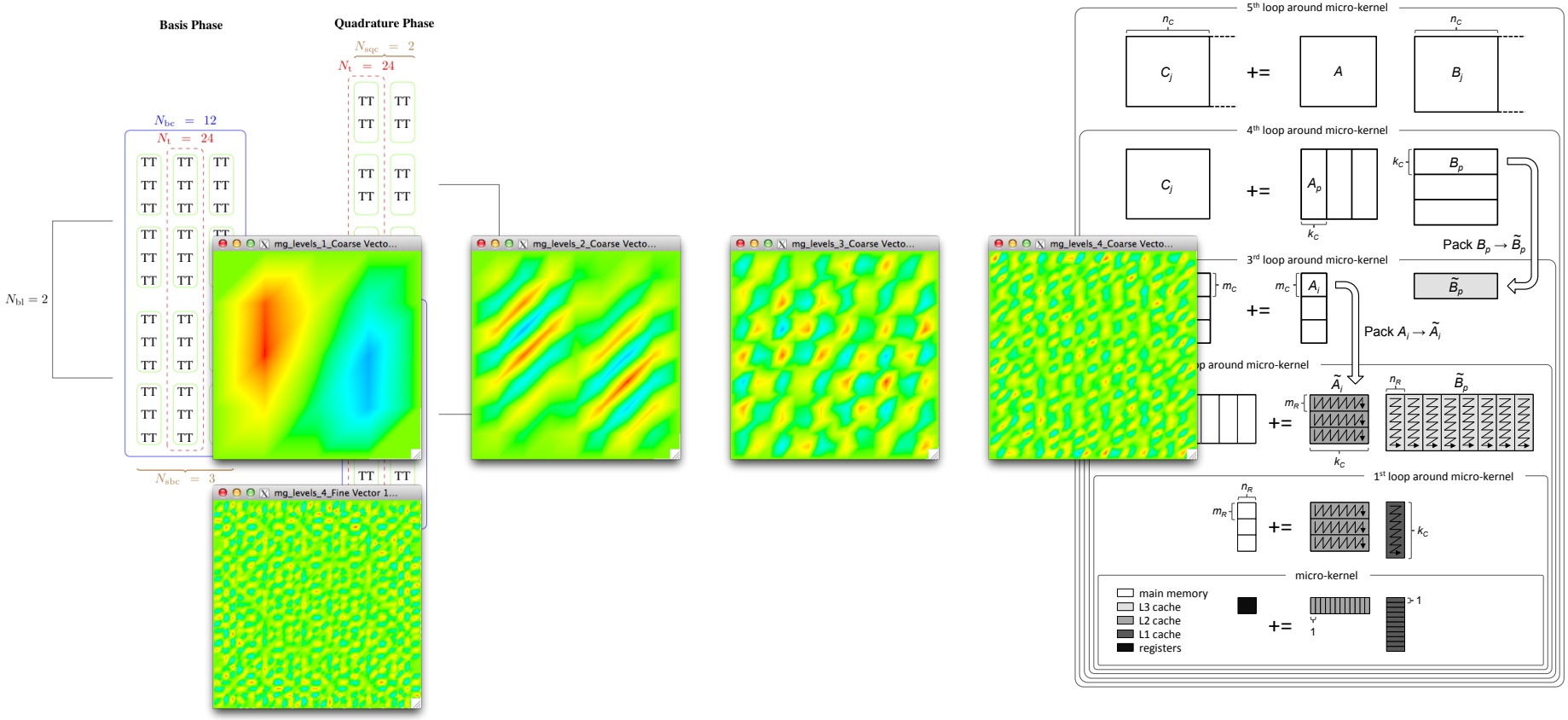

Libraries Accumulate Best Practices

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Classical Gram-Schmidt orthogonalization with selective reorthogonalization

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Eigen-estimation for AMG with Krylov bootstrap

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Classical Gram-Schmidt orthogonalization with selective reorthogonalization

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Improvement without code changes

Libraries Simplfy Determining Provenance

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Rather than making build-time choices,

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that must be plumbed through all levels

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with another layer of workflow scripts

Libraries Simplfy Determining Provenance

Rather than making build-time choices,
that must be plumbed through all levels
with another layer of workflow scripts
and brittle top-level interfaces,

Libraries Simplfy Determining Provenance

we use packages without modification,

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we use packages without modification,
compiled in a standard way

Libraries Simplfy Determining Provenance

we use packages without modification,
compiled in a standard way
and controlled entirely via runtime options.

Why PETSc?

- Dependability & Maintainability
- Portability & Robustness
- Performance & Scalability
- Optimality & Robustness
- Flexibility & Extensibility

Why PETSc?

- Dependability & Maintainability
  - Nearly 30 years of continuous development
- Portability & Robustness
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Why PETSc?

- Dependability & Maintainability
- Portability & Robustness
  - Tested at every supercomputer installation and 10,000+ users
- Performance & Scalability
- Optimality & Robustness
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- Dependability & Maintainability
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  - Many Gordon Bell Winners
- Optimality & Robustness
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Why PETSc?

- Dependability & Maintainability
- Portability & Robustness
- Performance & Scalability
- Optimality & Robustness
  - State-of-the-Art Linear and Nonlinear Solvers, Eigensolvers, Optimization Solvers, Timesteppers
- Flexibility & Extensibility

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Why PETSc?

- Dependability & Maintainability
- Portability & Robustness
- Performance & Scalability
- Optimality & Robustness
- Flexibility & Extensibility
  - More than 11,000 citations and hundreds of application packages
  - Aerodynamics, Arterial Flow, Corrosion, Combustion, Data Mining, Earthquake Mechanics, . . .

Alternatives to PETSc

There are other packages…

Alternatives to PETSc

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- DUNE, Hypre

Alternatives to PETSc

There are other packages…

- DUNE, Hypre
- Firedrake/FEniCS, FreeFEM, Deal.II

Alternatives to PETSc

There are other packages…

- DUNE, Hypre
- Firedrake/FEniCS, FreeFEM, Deal.II
- PyLith, Underworld, Salvus, SPECFEM, PFLOTRAN

PETSc Capabilities

- Parallel linear algebra (sparse and dense) [1]
- Linear [2] and nonlinear solvers [3]
- Timestepping [4]
- Optimization [5]
- Eigensolvers [6]
- Meshes
  - Cartesian
  - Structured adaptive [7]
  - Unstructured adaptive [8]
- Discretization support
  - Finite Difference
  - Finite Element [9]
  - Finite Volume [10]
- Portability (GPUs) [11]
- Profiling and debugging [12]

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Getting More Help

- https://petsc.org [13]
- Hyperlinked documentation
  - Sphinx and PDF Manual [14]
  - Manual pages for every method
  - HTML of example code (linked to manual pages)
- New Sphinx pages for manuals and tutorials
- FAQ
- Full support at petsc-maint@mcs.anl.gov

Outline

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- Hands-On Examples
  - Block Preconditioners
  - Multigrid
  - Nonlinear Preconditioning
  - Unstructured Mesh Creation*
  - ML*
  - Optimization*

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 ja
```

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

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 ga
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type ja
```

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

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 multiplicativ
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type ga
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type ja
```

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

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 multiplicativ
 -pc_fieldsplit_0_fields 1 -pc_fieldsplit_1_fields 0
 -fieldsplit_velocity_ksp_type preonly -fieldsplit_velocity_pc_type ga
 -fieldsplit_pressure_ksp_type preonly -fieldsplit_pressure_pc_type ja
```

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

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 ga
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type no
```

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

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 ga
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type no
```

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

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 ga
 -fieldsplit_pressure_ksp_type minres  -fieldsplit_pressure_pc_type no
```

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

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_pc_type
 -fieldsplit_pressure_ksp_max_it 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 jaco
```

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

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 jaco
 -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
```

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

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
```

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

Outline

- Hands-On Examples
  - Block Preconditioners
  - Multigrid
  - Nonlinear Preconditioning
  - Unstructured Mesh Creation*
  - ML*
  - Optimization*

Why not use 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`

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

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

Full Multigrid

The Full Multigrid algorithm (FMG)

- V-cycle at each level,
- then interpolate to the next finer grid
- Can solve to discretization error with a *single* iteration

Full Multigrid Work

$$
\begin{aligned}
C_{FMG} &= \left(1 + \frac{1}{2^d} + \frac{1}{2^{2d}} + \ldots\right) C_V \\
&= \sum_{n=0}^{\infty} \frac{1}{2^{nd}} C_V \\
&= \frac{2^d}{2^d - 1} C_V \\
&= \left(\frac{2^d}{2^d - 1}\right)^2 C_{\text{twolevel}}.
\end{aligned}
$$

Full Multigrid Work

$$
\begin{aligned}
C_{FMG} &= \left(1 + \frac{1}{2^d} + \frac{1}{2^{2d}} + \ldots\right) C_V \\
&= \sum_{n=0}^{\infty} \frac{1}{2^{nd}} C_V \\
&= \frac{2^d}{2^d - 1} C_V \\
&= \left(\frac{2^d}{2^d - 1}\right)^2 C_{\text{twolevel}}.
\end{aligned}
$$

1D FMG is $2 \times C_V$, 3D FMG is $\frac{8}{7} \times C_V$

Full Multigrid Accuracy

Suppose we have an order α method,

$$\|x - x_h\| < Ch^{\alpha}$$

FD and P_1 both have $\alpha = 2$

Full Multigrid Accuracy

E_d Discretization Error

E_a Algebraic Error

Choose iterative tolerance so that

$$E_a = rE_d \qquad r < 1$$

and

$$E \leq E_d + E_a = (1 + r)Ch^{\alpha}$$

Full Multigrid Accuracy

Suppose

- Finish V-cycle for $2h$ grid,
- Use as coarse correction for h grid
- Perform final V-cycle for h grid
- Need V-cycle error reduction factor η to get r reduction in E_a

Full Multigrid Accuracy

$$
\begin{aligned}
\eta E_a &< rCh^\alpha \\
\eta \left(E - E_d\right) &< rCh^\alpha \\
\eta \left((1+r)C(2h)^\alpha - Ch^\alpha\right) &< rCh^\alpha \\
\eta \left((1+r)2^\alpha - 1\right) &< r \\
\eta &< \frac{1}{2^\alpha + \frac{2^\alpha - 1}{r}}.
\end{aligned}
$$

If $\alpha = 2$ and $r = \frac{1}{2}$, then $\eta < \frac{1}{10}$.

Full Multigrid Experiment

V-cycle

```
./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
-ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short
```

gives

```
0 SNES Function norm 0.0287773
0 KSP Residual norm 0.793727
1 KSP Residual norm 0.00047526
2 KSP Residual norm 4.18007e-06
3 KSP Residual norm 1.1668e-07
4 KSP Residual norm 3.25952e-09
5 KSP Residual norm 7.274e-11
1 SNES Function norm 2.251e-10
N: 625 error l2 1.21529e-13 inf 9.53484e-12
```

Full Multigrid Experiment

V-cycle

```
./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
-ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short
```

and it changes little if we refine six more times

```
0 SNES Function norm 0.000455131
0 KSP Residual norm 50.6842
1 KSP Residual norm 0.00618427
2 KSP Residual norm 9.87833e-07
3 KSP Residual norm 2.99517e-09
1 SNES Function norm 2.83358e-09
N: 2362369 error l2 1.28677e-15 inf 7.68693e-12
```

Full Multigrid Experiment

FMG

```
./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
 -ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short
 -pc_mg_type full
```

We do not seem to see the convergence acceleration

```
0 SNES Function norm 0.0287773
0 KSP Residual norm 0.799687
1 KSP Residual norm 6.95292e-05
2 KSP Residual norm 1.50836e-06
3 KSP Residual norm 2.62524e-08
4 KSP Residual norm 6.184e-10
5 KSP Residual norm 1.275e-11
1 SNES Function norm 3.757e-11
N: 625 error l2 2.1428e-14 inf 1.80611e-12
```

Full Multigrid Experiment

FMG

```
./ex5 -mms 1 -par 0.0 -da_refine 3 -snes_type newtonls -snes_max_it 1
 -ksp_rtol 1e-10 -pc_type mg -snes_monitor_short -ksp_monitor_short
 -pc_mg_type full
```

although its a little more apparent as we refine,

```
0 SNES Function norm 0.000455131
0 KSP Residual norm 51.2
1 KSP Residual norm 2.92416e-06
2 KSP Residual norm 3.76404e-09
1 SNES Function norm 8.50096e-09
N: 2362369 error l2 1.70304e-15 inf 6.22476e-11
```

Full Multigrid Experiment

Script

```
#! /usr/bin/env python
import argparse
import subprocess
import numpy as np

parser = argparse.ArgumentParser(
description = 'CAAM 519 FMG',
epilog = 'For more information, visit http://www.mcs.anl.gov/petsc',
formatter_class = argparse.ArgumentDefaultsHelpFormatter)
parser.add_argument('--kmax', type=int, default=5,
                    help='The number of doublings to test')
parser.add_argument('--save', action='store_true', default=False,
                    help='Save the figures')
args = parser.parse_args()

sizesA = []
sizesB = []
errorA = []
errorB = []
```

Full Multigrid Experiment

Script

```
for k in range(args.kmax):
options = ['-snes_type', 'newtonls', '-snes_max_it', '1', '-da_refine'
           '-par', '0.0', '-ksp_atol', '1e-1', '-mms', '1',
           '-pc_type', 'mg', '-pc_mg_type', 'multiplicative',
           '-mg_levels_ksp_max_it', '5']
cmd = './ex5 '+' '.join(options)
out = subprocess.check_output(['./ex5']+options).split(' ')
# This is l_2, out[6] is l_infty
sizesA.append(int(out[1]))
errorA.append(float(out[4]))
for k in range(args.kmax):
options = ['-snes_type', 'newtonls', '-snes_max_it', '1', '-da_refine'
           '-par', '0.0', '-ksp_atol', '1e-1', '-mms', '1',
           '-pc_type', 'mg', '-pc_mg_type', 'full',
           '-mg_levels_ksp_max_it', '5']
cmd = './ex5 '+' '.join(options)
out = subprocess.check_output(['./ex5']+options).split(' ')
# This is l_2, out[6] is l_infty
sizesB.append(int(out[1]))
errorB.append(float(out[4]))
```

Full Multigrid Experiment

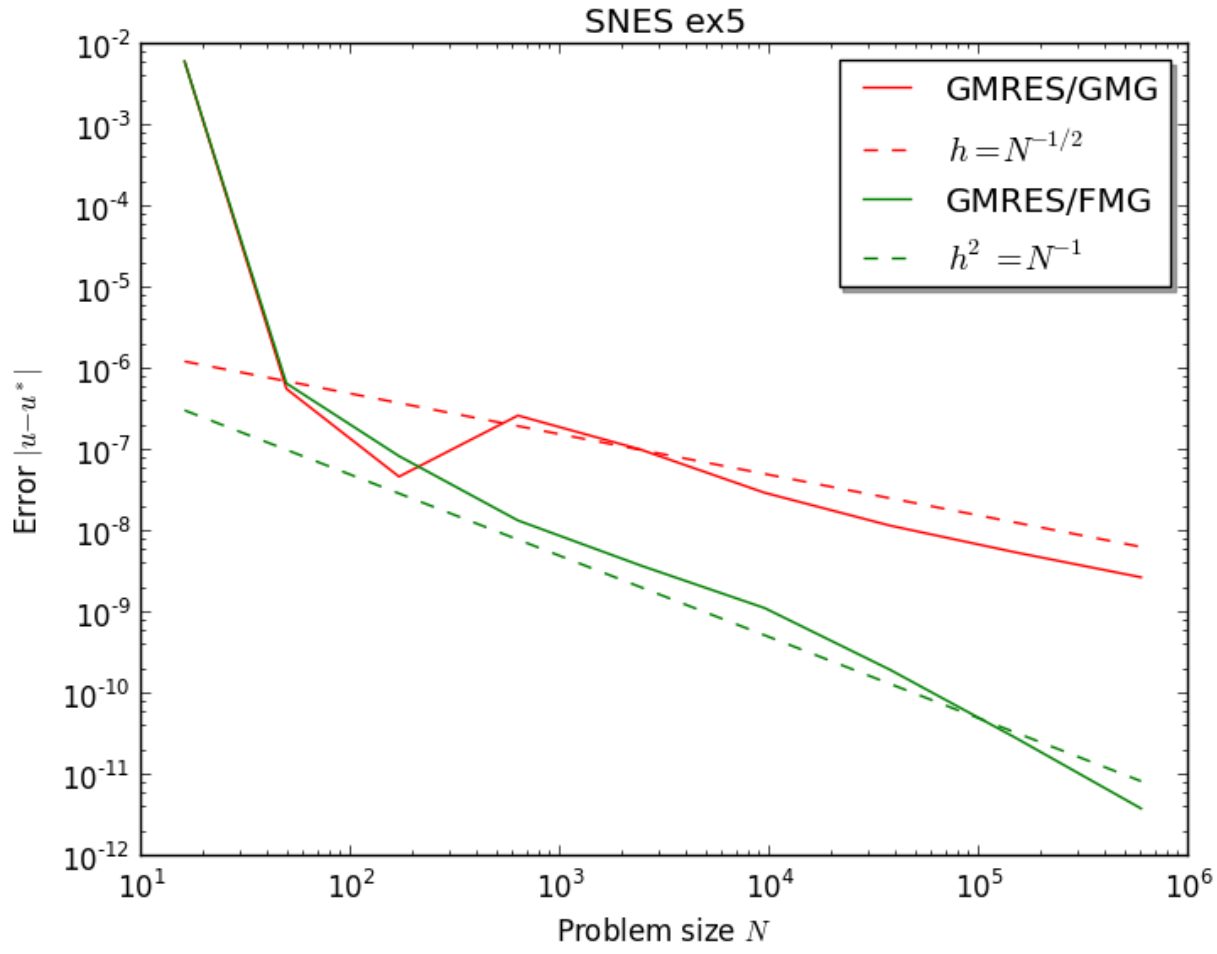
Script

```
SA = np.array(sizesA)
SB = np.array(sizesB)

from pylab import legend,plot,loglog,show,title,xlabel,ylabel,savefig
loglog(SA, errorA, 'r', SA, 5e-6 * SA ** -0.5, 'r--',
       SB, errorB, 'g', SB, 5e-6 * SB ** -1.,  'g--')
title('SNES ex5')
xlabel('Problem size $N$')
ylabel('Error $\|u - u^*\|$')
legend(['GMRES/GMG', '$h = N^{-1/2}$', 'GMRES/FMG', '$h^2 = N^{-1}$'],
       'upper right', shadow = True)
if args.save:
savefig('fmg.png')
else:
show()
```

Full Multigrid Experiment

Comparison



Outline

Hands-On Examples

- Block Preconditioners
- Multigrid
- Nonlinear Preconditioning
- Unstructured Mesh Creation*
- ML*
- Optimization*

Alternate Version

Excellent version by
Richard Mills

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
```

$$
\begin{aligned}
-\Delta U - \partial_y \Omega &= 0 \\
-\Delta V + \partial_x \Omega &= 0 \\
-\Delta \Omega + \nabla \cdot ([U\Omega, V\Omega]) - \mathrm{Gr}\, \partial_x T &= 0 \\
-\Delta T + \mathrm{Pr}\, \nabla \cdot ([UT, VT]) &= 0
\end{aligned}
$$

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 iteratio
```

Driven Cavity Problem

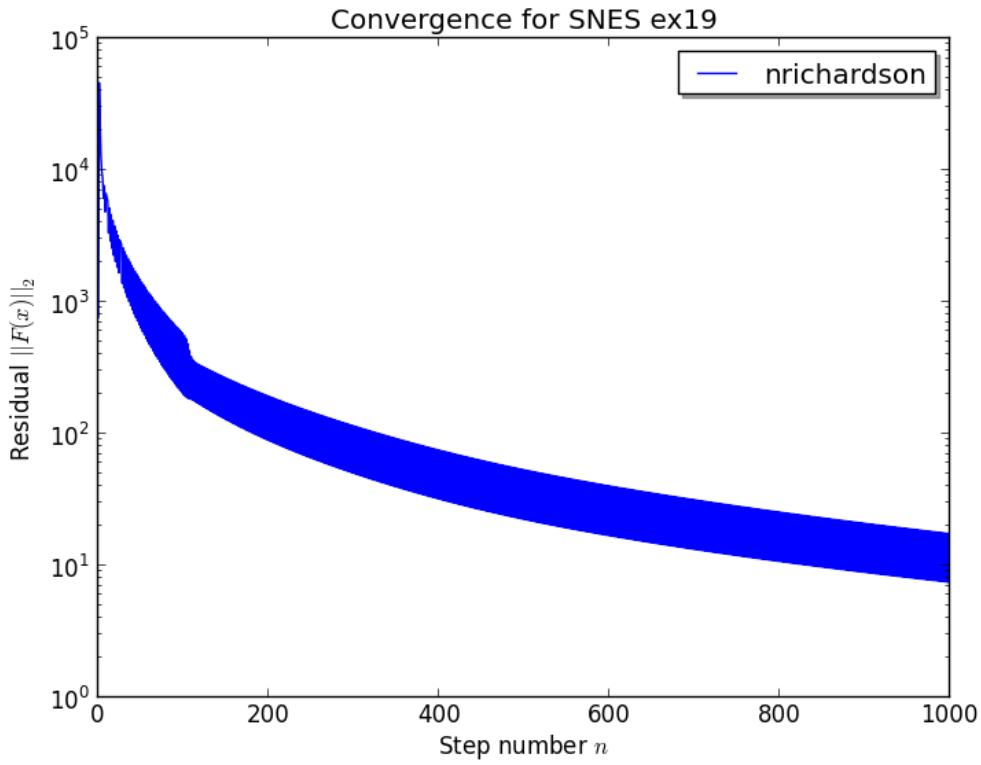
SNES ex19.c

```
./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
 ...
```

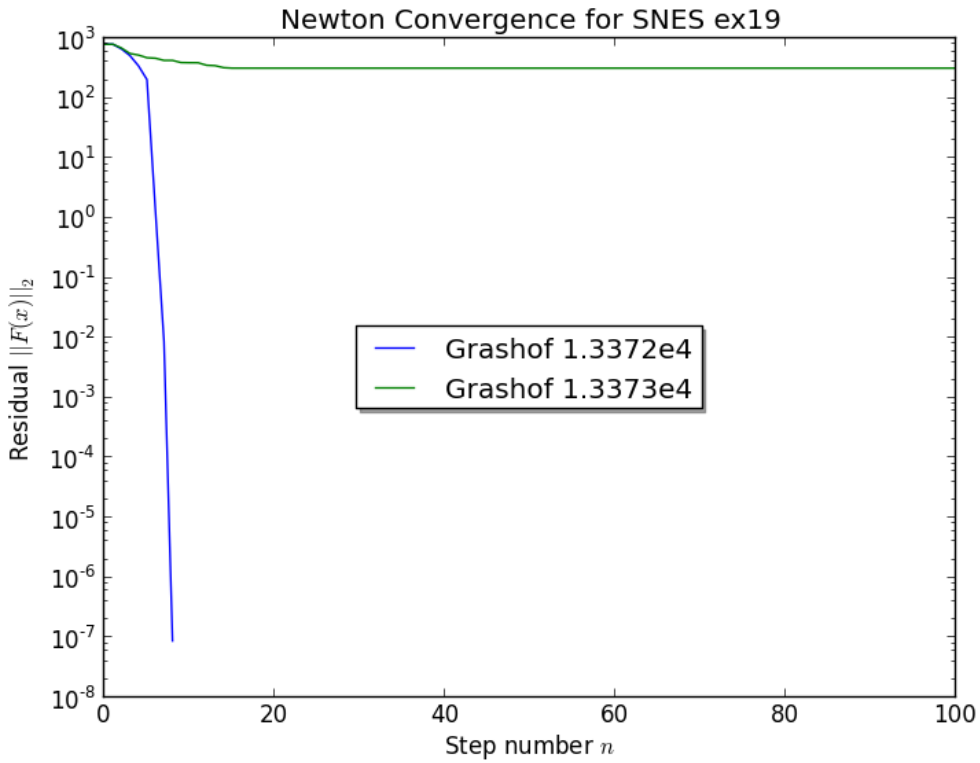
Deceleration of Convergence

```
./ex19 -lidvelocity 100 -grashof 1.3372e2
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type nrichardson -snes_linesearch_type cp -snes_max_it 10000
  -snes_monitor draw::draw_lg
```



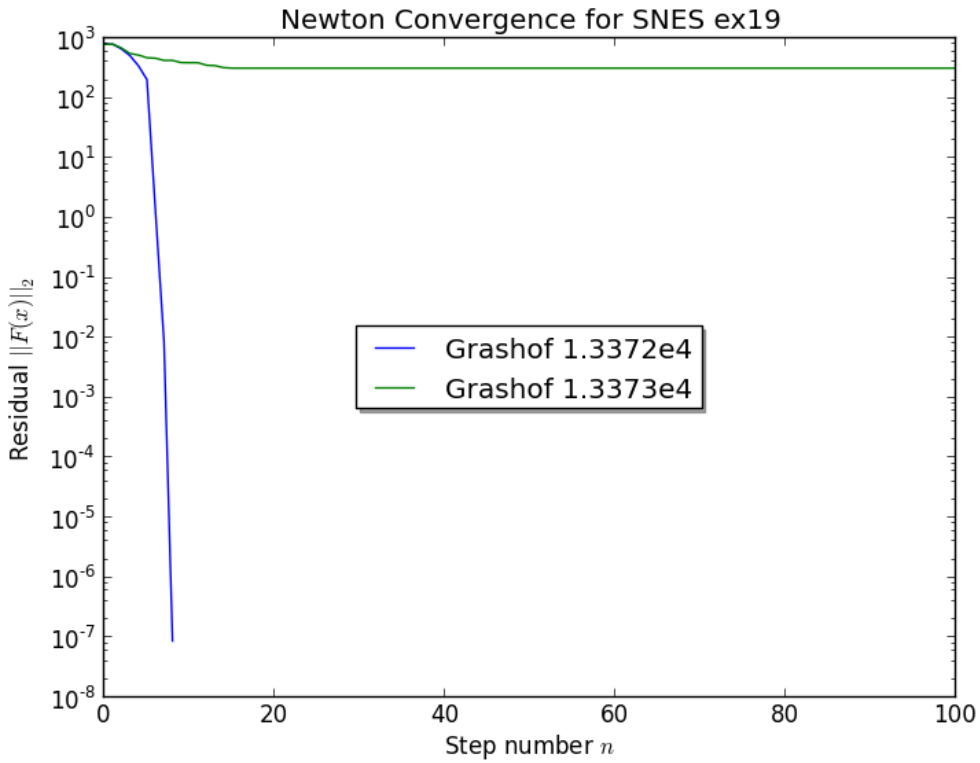
Stagnation of Newton

```
./ex19 -lidvelocity 100 -grashof 1.3372e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 100 -pc_type lu
```



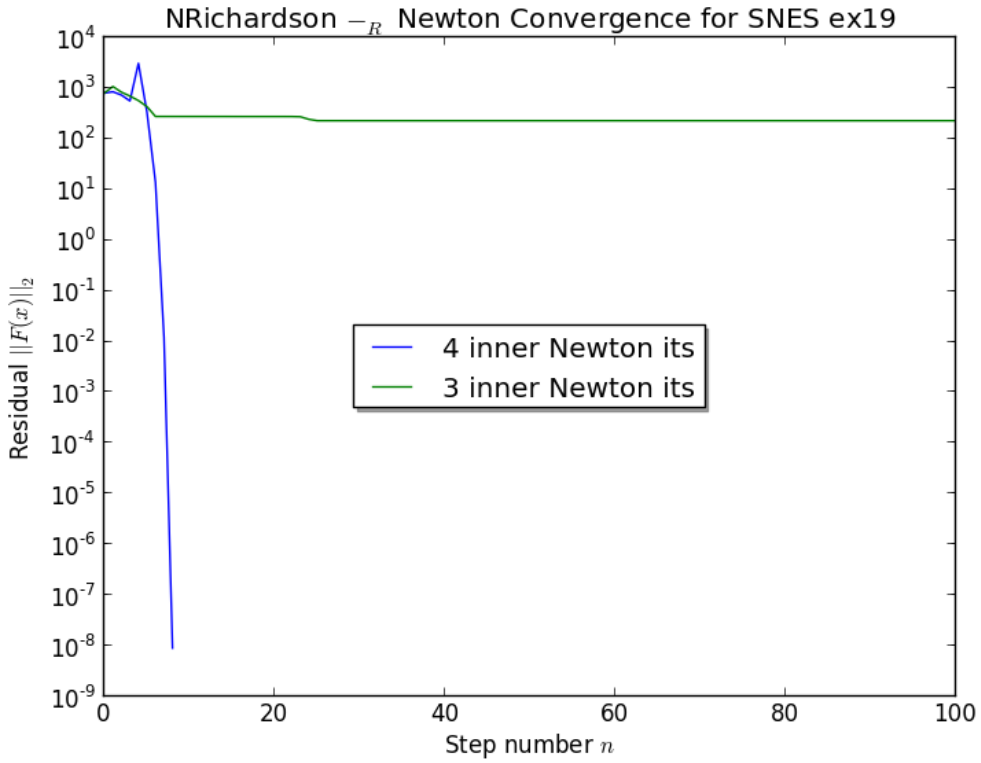
Stagnation of Newton

```
./ex19 -lidvelocity 100 -grashof 1.3373e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 100 -pc_type lu
```



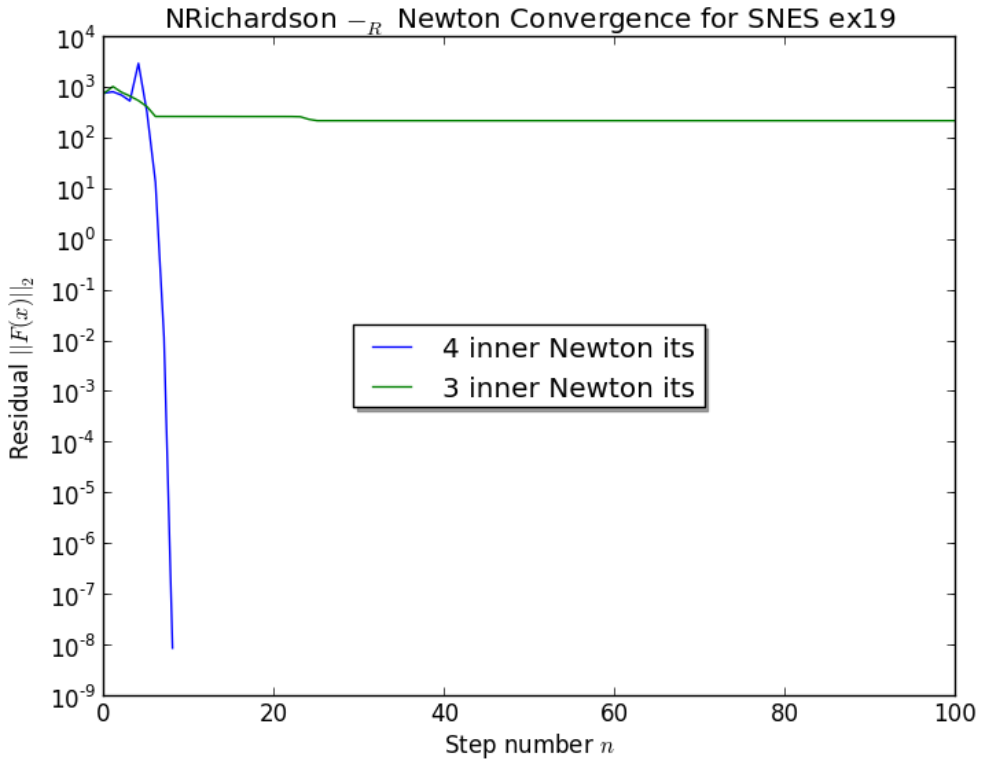
Preconditioning NRichardson with Newton

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type nrichardson -snes_max_it 200
  -npc_snes_type newtonls -npc_snes_max_it 1 -npc_pc_type lu
  -snes_monitor draw::draw_lg -snes_monitor_pause_final
```



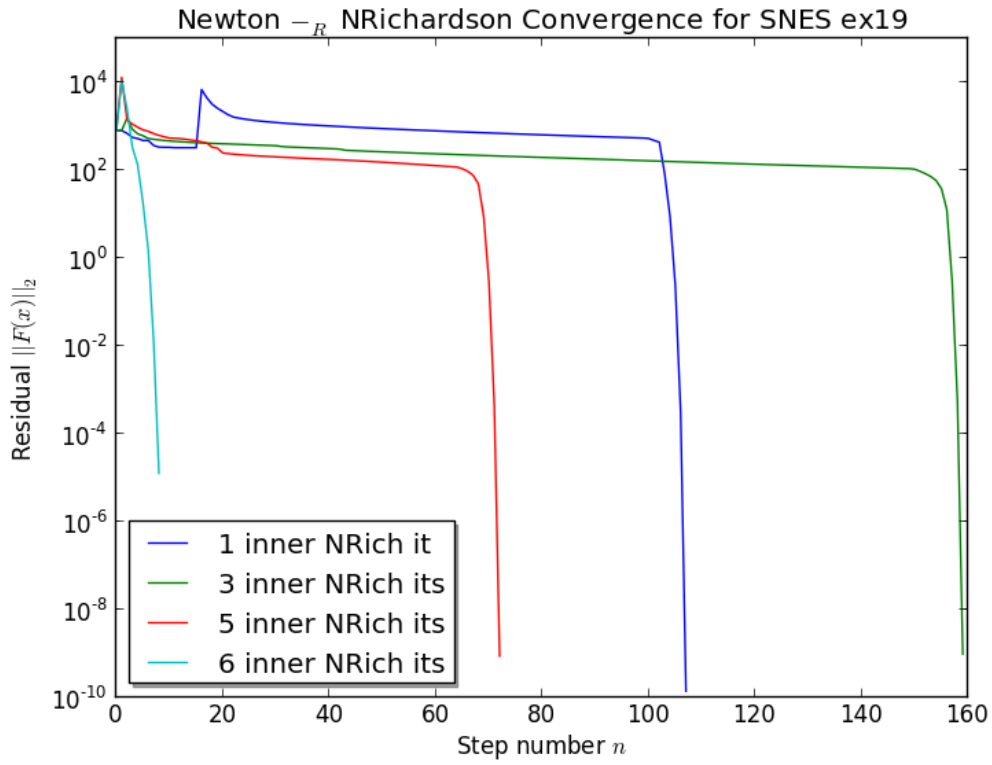
Preconditioning NRichardson with Newton

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type nrichardson -snes_max_it 200
  -npc_snes_type newtonls -npc_snes_max_it 2 -npc_pc_type lu
  -snes_monitor draw::draw_lg -snes_monitor_pause_final
```



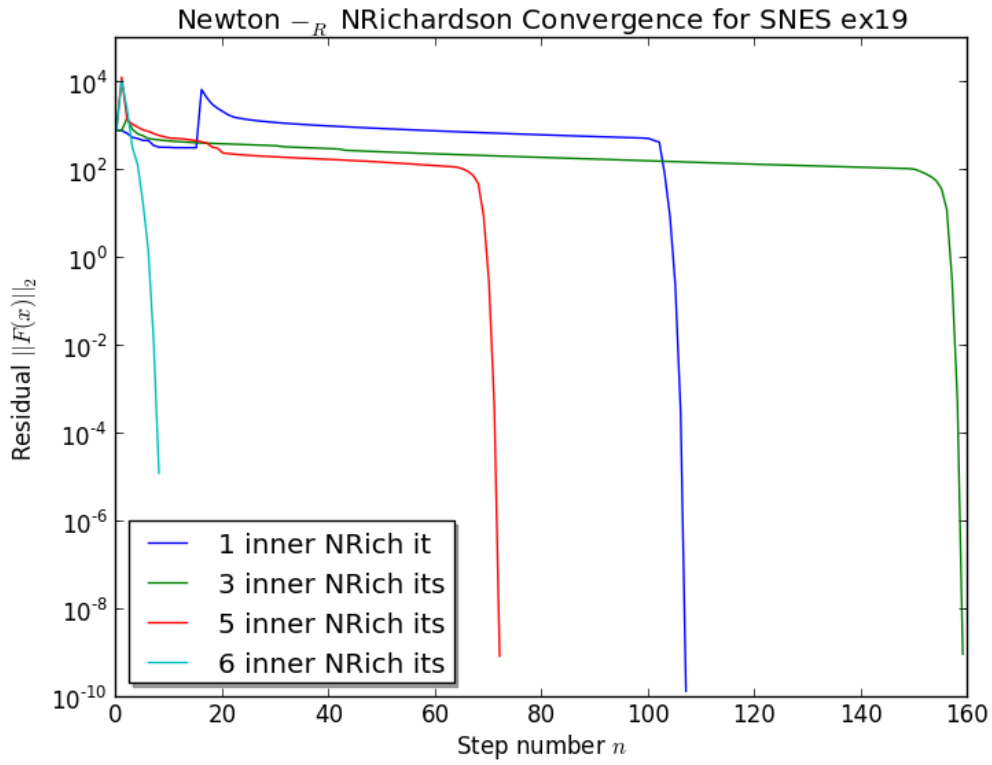
Preconditioning Newton with NRichardson

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 1
```



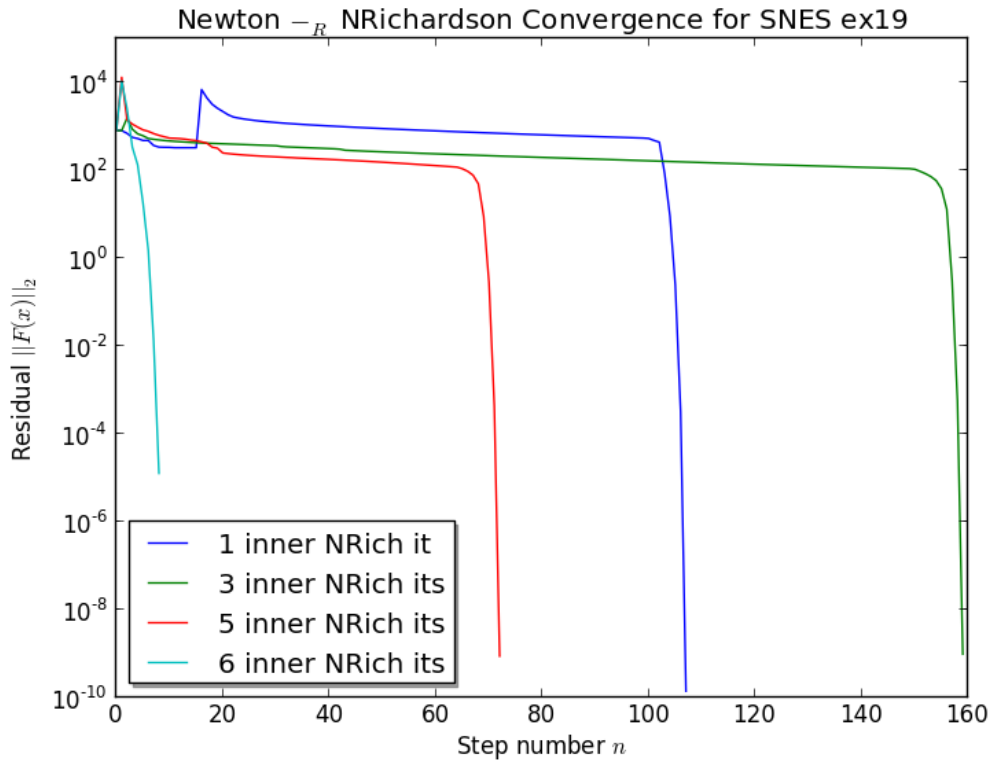
Preconditioning Newton with NRichardson

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 3
```



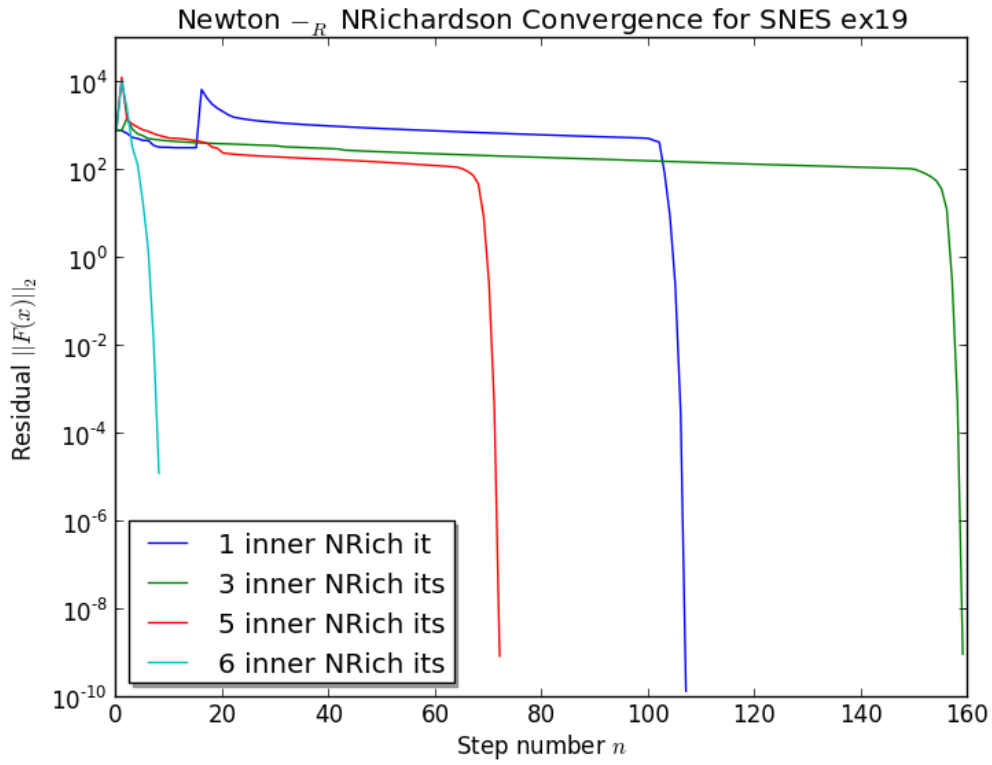
Preconditioning Newton with NRichardson

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 5
```



Preconditioning Newton with NRichardson

```
./ex19 -lidvelocity 100 -grashof 1.35e4
  -da_grid_x 16 -da_grid_y 16 -da_refine 2
  -snes_type newtonls -snes_max_it 1000 -pc_type lu
  -npc_snes_type nrichardson -npc_snes_max_it 6
```



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
  :
 61 SNES Function norm 320.325
 62 SNES Function norm 320.325
 63 SNES Function norm 320.325 21 SNES Function norm 585.143
  :
```

Nonlinear Preconditioning

```
./ex19 -lidvelocity 100 -grashof 5e4 -da_refine 4 -snes_monitor_short
 -snes_type fas -snes_converged_reason
 -fas_levels_snes_type ngs -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
  ...cycles without convergence...
```

Nonlinear Preconditioning

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


lid velocity = 100, prandtl # = 1, grashof # = 50000
  0 SNES Function norm 1228.95
  1 SNES Function norm 552.271
    Nonlinear npc_fas_coarse_ solve did not converge due to DIVERGED_M
  2 SNES Function norm 355.543
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_FNORM_R
  :
  :
  38 SNES Function norm 3.74123e-05
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_SNORM_R
  39 SNES Function norm 2.61273e-05
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_SNORM_R
  40 SNES Function norm 1.16528e-05
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 4
```

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 npc_fas_coarse_ solve converged due to CONVERGED_FNORM_R
  1 SNES Function norm 538.605
    Nonlinear npc_fas_coarse_ solve did not converge due to DIVERGED_M
  2 SNES Function norm 418.638
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_FNORM_R
⋮


  24 SNES Function norm 0.000119837
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_FNORM_R
  25 SNES Function norm 2.77111e-05
    Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_SNORM_R
  26 SNES Function norm 1.11942e-05
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 2
```

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_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 npc_fas_levels_4_ solve converged due to CONVERGED_ITS i
    :
        Nonlinear npc_fas_coarse_ solve converged due to CONVERGED_SNO
    :
  1 SNES Function norm 2.88944
  2 SNES Function norm 0.0803355
  3 SNES Function norm 0.0131489
  4 SNES Function norm 0.00118131
  5 SNES Function norm 1.65056e-05
  6 SNES Function norm 9.6292e-09
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 6
```

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 ngs -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 538.539
  2 SNES Function norm 163.178
  3 SNES Function norm 49.5499
  4 SNES Function norm 11.5314
  5 SNES Function norm 0.182861
  6 SNES Function norm 0.00148081
  7 SNES Function norm 1.49034e-07
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 544.417
  2 SNES Function norm 18.2329
  3 SNES Function norm 1.05348
  4 SNES Function norm 0.00460528
  5 SNES Function norm 1.40734e-05
  6 SNES Function norm 3.07181e-08
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations
```

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 Algebraic Solvers,
Peter Brune, Matthew Knepley, Barry Smith, and Xuemin Tu,

SIAM Review, **57**(4), 535–565, 2015.

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

Outline

- Hands-On Examples
  - Block Preconditioners
  - Multigrid
  - Nonlinear Preconditioning
  - Unstructured Mesh Creation*
  - ML*
  - Optimization*

Plex Tutorial ex2: source

Outline

- Hands-On Examples
  - Block Preconditioners
  - Multigrid
  - Nonlinear Preconditioning
  - Unstructured Mesh Creation*
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  - Optimization*

PetscRegressor Tutorial and Notebook

Outline

- Hands-On Examples
  - Block Preconditioners
  - Multigrid
  - Nonlinear Preconditioning
  - Unstructured Mesh Creation*
  - ML*
  - Optimization*

Optimization Tutorial

Outline

Parallel Computing is Not Magic

Performance controlled by bandwidth and latency

- Bandwidth is determined by nodes, not cores
- Usually saturates with less than half the cores
- STREAM benchmark is a good measure

Parallel Computing is Not Magic

Most effective for

- increasing problem size (weak scaling),
- not faster solutions (strong scaling).

Strong scalability is limited by

- Ahmdahl's Law, but
- bandwidth saturation is often confused with this.

GPUs are Not Magic

Performance improvement is often quite limited:

- Bandwidth $<$ 10x of a top end CPU

  AMD EPYC 9000 1 TB/s, NVIDIA Grace 800 GB/s
  AMD MI325X 6 TB/s, NVIDIA Blackwell 8 TB/s

- Very high memory latency,
- Steep fall off for smaller loads

Toolchain is rapidly evolving and not robust.

Machine Learning is Not Magic

The sweet spot for Deep Neural Networks is

- many parameters (millions), and
- no knowledge of what is important.

Machine Learning is Not Magic

	Few Parameters	Many Parameters
Some idea	Logistic Reg.	Bayesian Inference
No idea	Logistic Reg.	Neural Networks

References I

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[2] Jed Brown, Matthew G. Knepley, David A. May, Lois C. McInnes, and Barry F. Smith. "Composable linear solvers for multiphysics". In: Proceeedings of the 11th International Symposium on Parallel and Distributed Computing (ISPDC 2012). IEEE Computer Society, 2012, pp. 55–62. DOI: 10.1109/ISPDC.2012.16.

[3] Peter R. Brune, Matthew G. Knepley, Barry F. Smith, and Xuemin Tu. "Composing Scalable Nonlinear Algebraic Solvers". In: SIAM Review 57.4 (2015). http://www.mcs.anl.gov/papers/P2010-0112.pdf, pp. 535–565. DOI: 10.1137/130936725. URL: http://www.mcs.anl.gov/papers/P2010-0112.pdf.

[4] Shrirang Abhyankar, Jed Brown, Emil Constantinescu, Debojyoti Ghosh, and Barry F. Smith. PETSc/TS: A Modern Scalable DAE/ODE Solver Library. Preprint ANL/MCS-P5061-0114. ANL, Jan. 2014.

[5] Steven J Benson and Todd S Munson. "Flexible complementarity solvers for large-scale applications". In: Optimization Methods and Software 21.1 (2006), pp. 155–168.

[6] Carmen Campos, José E. Román, Eloy Romero, Andrés Tomás, Vicente Hernández, and Vicent Vidal. "SLEPc Website". Scalable Library for Eigenvalue Problem Computations. URL: http://slepc.upv.es/.

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Outline

Outline

Downloading PETSc

- There is a Git repository
- The latest tarball is on the PETSc site: https://web.cels.anl.gov/projects/petsc/download/release-snapshots/
- There is a pip package (`pip install petsc petsc4py`)
- There is a Debian package (`aptitude install petsc-dev`)

Cloning PETSc

- The full development repository is open to the public
  - https://gitlab.com/petsc/petsc/
- Why is this better?
  - You can clone to any release (or any specific ChangeSet)
  - You can easily rollback changes (or releases)
  - You can get fixes from us the same day
  - You can easily submit changes using a pull request
- All releases are just tags:
  - Source at tag v3.18.0

Unpacking PETSc

- Just clone development repository
  - `git clone http://gitlab.com/petsc/petsc.git`
  - `git checkout -rv3.24.0`

or

- Unpack the tarball
  - `tar xzf petsc.tar.gz`

Exercise 1

Download and Unpack PETSc!

Outline

Configuring PETSc

- Set `$PETSC_DIR` to the installation root directory
- Run the configuration utility
  - `$PETSC_DIR/configure`
  - `$PETSC_DIR/configure --help`
  - `$PETSC_DIR/configure --download-mpich`
  - `$PETSC_DIR/configure --prefix=/usr`
- There are many examples in `$PETSC_DIR/config/examples`
- Config files in `$PETSC_DIR/$PETSC_ARCH/lib/petsc/conf`
  - Config header in `$PETSC_DIR/$PETSC_ARCH/include`
  - `$PETSC_ARCH` has a default if not specified

Configuring PETSc

- You can easily reconfigure with the same options
  -
    ```
    ./$PETSC_ARCH/lib/petsc/conf/reconfigure-$PETSC_ARCH.py
    ```
- Can maintain several different configurations
  -
    ```
    ./configure -PETSC_ARCH=arch-linux-opt --with-debugging=0
    ```
- All configuration information is in the logfile
  - `./$PETSC_ARCH/lib/petsc/conf/configure.log`
  - ALWAYS send this file with bug reports

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen
–download-p4est –download-egads

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen
–download-p4est –download-egads

–download-eigen –download-pragmatic
–download-metis –download-parmetis

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen
–download-p4est –download-egads

–download-eigen –download-pragmatic
–download-metis –download-parmetis

–download-hdf5 –download-netcdf
–download-pnetcdf –download-exodusii

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen
–download-p4est –download-egads

–download-eigen –download-pragmatic
–download-metis –download-parmetis

–download-hdf5 –download-netcdf
–download-pnetcdf –download-exodusii

–download-ml –download-superlu –download-superlu_dist
–download-scalapack –download-mumps

Configuring PETSc for FEM

$PETSC_DIR/configure

–download-triangle –download-ctetgen
–download-p4est –download-egads

–download-eigen –download-pragmatic
–download-metis –download-parmetis

–download-hdf5 –download-netcdf
–download-pnetcdf –download-exodusii

–download-ml –download-superlu –download-superlu_dist
–download-scalapack –download-mumps

–download-fftw –download-slepc –download-bamg

Configuring PETSc for Acclerators

```
$PETSC_DIR/configure
        –with-precision=single
```

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–with-cuda

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–with-cuda

–with-cudac=’nvcc -m64’ –with-cuda-arch=sm_10

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–with-opencl

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–with-opencl

–with-opencl-include=/System/Library/Frameworks/OpenCL.framework/Headers/

–with-opencl-lib=/System/Library/Frameworks/OpenCL.framework/OpenCL

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–download-kokkos –download-kokkos-kernels

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–with-cuda

–download-kokkos –download-kokkos-kernels

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–download-kokkos –download-kokkos-kernels

–with-hip

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–download-kokkos –download-kokkos-kernels

–with-sycl

Configuring PETSc for Acclerators

$PETSC_DIR/configure

–with-precision=single

–download-kokkos –download-kokkos-kernels

–with-openmp

Automatic Downloads

- Starting in 2.2.1, some packages are automatically
  - Downloaded
  - Configured and Built (in `$PETSC_DIR/externalpackages`)
  - Installed with PETSc
- Currently works for
  - petsc4py, mpi4py
  - PETSc documentation utilities (Sowing, c2html)
  - BLAS, LAPACK, Elemental, ScaLAPACK
  - GMP, MPFR
  - ConcurrencyKit, hwloc
  - MPICH, OpenMPI
  - ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
  - SuiteSparse, MUMPS, SuperLU, SuperLU_Dist, PaStiX, Pardiso
  - SLEPc, HYPRE, ML
  - BLOPEX, FFTW, STRUMPACK, SPAI, CUSP, Sundials
  - Triangle, TetGen, p4est, Pragmatic
  - HDF5, NetCDF, ExodusII
  - AfterImage, gifLib, libjpeg, opengl

Exercise 2

Configure your downloaded PETSc.

Outline

Building PETSc

- There is now One True Way to build PETSc:
  - `make`
  - `make install` if you configured with `--prefix`
  - Check build when done with `make check`
- Can build multiple configurations
  - `PETSC_ARCH=arch-linux-opt make`
  - Libraries are in `$PETSC_DIR/$PETSC_ARCH/lib/`
- Complete log for each build is in logfile
  - `./$PETSC_ARCH/lib/petsc/conf/make.log`
  - ALWAYS send this with bug reports

Exercise 3

Build your configured PETSc.

Exercise 4

Reconfigure PETSc to use ParMetis.

1. `linux-debug/lib/petsc/conf/reconfigure-linux-debug.py`
   - `--PETSC_ARCH=arch-linux-parmetis`
   - `--download-metis --download-parmetis`
2. `PETSC_ARCH=linux-parmetis make`
3. `PETSC_ARCH=linux-parmetis make check`