The Portable Extensible Toolkit for Scientific Computing

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ARGONNE NATIONAL LABORATORY

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assess solver performance,

and optimize solvers
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Outline

Controlling PETSc

All of PETSc can be controlled by options

`-ksp_type gmres`

`-start_in_debugger`

All objects can have a prefix, `-velocity_pc_type jacobi`

All PETSc options can be namespaced

`-sub_ksp_type bicg`

`-fieldsplit_1_pc_type jacobi`

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Examples

We will illustrate options using

PETSc SNES ex5, located at

`$PETSC_DIR/src/snes/examples/tutorials/ex5.c`

and

PETSc SNES ex62, located at

`$PETSC_DIR/src/snes/examples/tutorials/ex62.c`

Outline

1. Controlling the Solver
2. Where do I begin?
3. How do I improve?
4. Debugging
5. Examples

Nonlinear Systems

I am not going to discuss nonlinear systems today,

however if Newton is failing,

contact

petsc-maint@mcs.anl.gov

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What is a Krylov solver?

A Krylov solver builds a small model of a linear operator A, using a subspace defined by

$$\mathcal{K}(A, r) = \mathrm{span}\{r, Ar, A^2 r, A^3 r, \ldots\}$$

where r is the initial residual.

The small system is sovled directly, and the solution is projected back to the original space.

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What Should I Know About Krylov Solvers?

- They can handle *low-mode* errors
- They need preconditioners
- They do a lot of inner products

What is a Preconditioner?

A preconditioner M changes a linear system,

$$M^{-1}Ax = M^{-1}b$$

so that the effective operator is $M^{-1}A$, which is hopefully better for Krylov methods.

- Preconditioner should be inexpensive
- Preconditioner should accelerate convergence

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Always start with LU

Always, always start with LU:

- No iterative tolerance
- (Almost) no condition number dependence
- Check for accidental singularity

In parallel, you need a 3rd party package

- MUMPS (`--download-mumps`)
- SuperLU (`--download-superlu_dist`)

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What if LU fails?

LU will fail for

- Singular problems
- Saddle-point problems

For saddles use PC_FIELDSPLIT

- Separately solves each field
- Decomposition is automatic in PyLith
- Autodetect with -pc_fieldsplit_detect_saddle_point
- Exact with full Schur complement solve

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For saddles use `PC_FIELDSPLIT`

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- Autodetect with `-pc_fieldsplit_detect_saddle_point`
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3. How do I improve?
   - Look at what you have
   - Back off in steps

What solver did you use?

Use `-snes_view` or `-ksp_view` to output a description of the solver:

```
KSP Object:         (fieldsplit_0_)         1 MPI processes
  type: fgmres
    GMRES: restart=100, using Classical (unmodified) Gram-
      Schmidt Orthogonalization with no iterative refinemen
    GMRES: happy breakdown tolerance 1e-30
  maximum iterations=1, initial guess is zero
  tolerances:  relative=1e-09, absolute=1e-50,
    divergence=10000
  right preconditioning
  has attached null space
  using UNPRECONDITIONED norm type for convergence test
```

What did the convergence look like?

Use `-snes_monitor` and `-ksp_monitor`, or `-log_summary`:

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Use `-snes_monitor` and `-ksp_monitor`, or `-log_summary`:

```
0 SNES Function norm 0.207564
1 SNES Function norm 0.0148968
2 SNES Function norm 0.000113968
3 SNES Function norm 6.9256e-09
4 SNES Function norm < 1.e-11
```

What did the convergence look like?

Use `-snes_monitor` and `-ksp_monitor`, or `-log_summary`:

```
0 KSP Residual norm 1.61409
    Residual norms for mg_levels_1_ solve.
    0 KSP Residual norm 0.213376
    1 KSP Residual norm 0.0192085
  Residual norms for mg_levels_2_ solve.
  0 KSP Residual norm 0.223226
  1 KSP Residual norm 0.0219992
    Residual norms for mg_levels_1_ solve.
    0 KSP Residual norm 0.0248252
    1 KSP Residual norm 0.0153432
  Residual norms for mg_levels_2_ solve.
  0 KSP Residual norm 0.0124024
  1 KSP Residual norm 0.0018736
1 KSP Residual norm 0.02282
```

What did the convergence look like?

Use `-snes_monitor` and `-ksp_monitor`, or `-log_summary`:

```
Event          Count       Time (sec)        Flops         Total
             Max Ratio  Max        Ratio   Max   Ratio Mflop/s
KSPSetUp        12 1.0 3.6259e-03 1.0 0.00e+00 0.0       0
KSPSolve         3 1.0 4.8937e-01 1.0 8.93e+05 1.0       2
SNESSolve        1 1.0 4.9477e-01 1.0 9.22e+05 1.0       2
```

Look at timing

Use `-log_summary`:

```
Event            Time (sec)        Flops        --- Global ---   Total
               Max       Ratio    Max   Ratio %T %f %M %L %R   MF/s
VecMDot     1.8904e-03 1.0 2.49e+04 1.0  0  3  0  0  0     13
MatMult     2.1026e-03 1.0 2.65e+05 1.0  0 29  0  0  0    126
PCApply     4.6001e-01 1.0 7.78e+05 1.0 58 84  0  0 64      2
KSPSetUp    3.6259e-03 1.0 0.00e+00 0.0  0  0  0  0  4      0
KSPSolve    4.8937e-01 1.0 8.93e+05 1.0 61 97  0  0 90      2
SNESSolve 4.9477e-01 1.0 9.22e+05 1.0 62100  0  0 92      2
```

Use `-log_summary_python` to get this information as a Python module

Look at timing

Use `-log_summary`:

Event	Time (sec)		Flops		--- Global ---					Total
	Max	Ratio	Max	Ratio	%T	%f	%M	%L	%R	MF/s
VecMDot	1.8904e-03	1.0	2.49e+04	1.0	0	3	0	0	0	13
MatMult	2.1026e-03	1.0	2.65e+05	1.0	0	29	0	0	0	126
PCApply	4.6001e-01	1.0	7.78e+05	1.0	58	84	0	0	64	2
KSPSetUp	3.6259e-03	1.0	0.00e+00	0.0	0	0	0	0	4	0
KSPSolve	4.8937e-01	1.0	8.93e+05	1.0	61	97	0	0	90	2
SNESSolve	4.9477e-01	1.0	9.22e+05	1.0	62	100	0	0	92	2

Use `-log_summary_python` to get this information as a Python module

Outline

3. How do I improve?
   - Look at what you have
   - Back off in steps

Weaken the KSP

GMRES $\Longrightarrow$ BiCGStab

- `-ksp_type bcgs`
- Less storage
- Fewer dot products (less work)
- Variants `-ksp_type bcgsl` and `-ksp_type ibcgs`

Complete Table of Solvers and Preconditioners

Weaken the PC

LU $\Longrightarrow$ ILU

- `-pc_type ilu`
- Less storage and work

In parallel,

- Hypre `-pc_type hypre -pc_hypre_type euclid`
- Block-Jacobi `-pc_type bjacobi -sub_pc_type ilu`
- Additive Schwarz `-pc_type asm -sub_pc_type ilu`

Default for MG smoother is Chebychev/SOR(2)

Weaken the PC

LU $\implies$ ILU

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Default for MG smoother is Chebychev/SOR(2)

Algebraic Multigrid (AMG)

- Can solve elliptic problems
  - Laplace, elasticity, Stokes
- Works for unstructured meshes
- `-pc_type gamg`, `-pc_type ml`, `-pc_type hypre -pc_hypre_type boomeramg`
- CRUCIAL to have an accurate near-null space
  - MatSetNearNullSpace()
  - PyLith provides this automatically
- Use `-pc_mg_log` to put timing in its own log stage

PC_FieldSplit

- Separate solves for block operators
  - Physical insight for subsystems
  - Have optimial PCs for simpler equations
  - Suboptions `fs_fieldsplit_0_*`
- Flexibly combine subsolves
  - Jacobi: `fs_pc_fieldsplit_type = additive`
  - Gauss-Siedel: `fs_pc_fieldsplit_type = multiplicative`
  - Schur complement: `fs_pc_fieldsplit_type = schur`

Stokes example

The common block preconditioners for Stokes require only options:

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

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type additive

-fieldsplit_0_pc_type ml
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

PC

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

Cohouet & Chabard, Some fast 3D finite element solvers for the generalized Stokes problem, 1988.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type multiplic
-fieldsplit_0_pc_type hypre
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type jacobi
-fieldsplit_1_ksp_type preonly
```

PC

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

Elman, Multigrid and Krylov subspace methods for the discrete Stokes equations, 1994.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type diag
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.
Olshanskii, Peters, and Reusken, Uniform preconditioners for a parameter dependent saddle point problem with application to generalized Stokes interface equations, 2006.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type lower
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur
-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly
-fieldsplit_1_pc_type none
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type upper
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.

Stokes example

The common block preconditioners for Stokes require only options:

```
-pc_type fieldsplit
-pc_field_split_type schur

-fieldsplit_0_pc_type gamg
-fieldsplit_0_ksp_type preonly

-fieldsplit_1_pc_type lsc
-fieldsplit_1_ksp_type minres
```

PC

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

```
-pc_fieldsplit_schur_factorization_type upper
```

May and Moresi, Preconditioned iterative methods for Stokes flow problems arising in computational geodynamics, 2007.
Kay, Loghin and Wathen, A Preconditioner for the Steady-State N-S Equations, 2002.
Elman, Howle, Shadid, Shuttleworth, and Tuminaro, Block preconditioners based on approximate commutators, 2006.

Stokes example

The common block preconditioners for Stokes require only options:

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

PC

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

Why us FGMRES?

Flexible GMRES (FGMRES) allows a different preconditioner at each step:

- Takes twice the memory
- Needed for iterative PCs
- Avoided sometimes with a careful PC choice

Outline

Correctness Debugging

- Automatic generation of tracebacks
- Detecting memory corruption and leaks
- Optional user-defined error handlers

Interacting with the Debugger

- Launch the debugger
  - `-start_in_debugger [gdb,dbx,noxterm]`
  - `-on_error_attach_debugger [gdb,dbx,noxterm]`
- Attach the debugger only to some parallel processes
  - `-debugger_nodes 0,1`
- Set the display (often necessary on a cluster)
  - `-display khan.mcs.anl.gov:0.0`

Debugging Tips

- Put a breakpoint in `PetscError()` to catch errors as they occur
- PETSc tracks memory overwrites at both ends of arrays
  - The `CHKMEMQ` macro causes a check of all allocated memory
  - Track memory overwrites by bracketing them with `CHKMEMQ`
- PETSc checks for leaked memory
  - Use `PetscMalloc()` and `PetscFree()` for all allocation
  - Print unfreed memory on `PetscFinalize()` with `-malloc_dump`
- Simply the best tool today is valgrind
  - It checks memory access, cache performance, memory usage, etc.
  - http://www.valgrind.org
  - Need `-trace-children=yes` when running under MPI

Outline

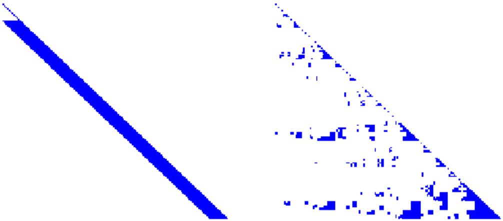
Try it out

```
$ cd $PETSC_DIR/src/snes/examples/tutorials && make ex5
```

- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view`
- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -mat_view_draw -draw_pause 0.5`
- `$ ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -mat_view_draw -draw_pause 0.5 -pc_type lu -pc_factor_mat_ordering_type natural`
- Use `-help` to find other ordering types

Sample output

```
0 SNES Function norm 1.139460779565e+00
Linear solve converged due to CONVERGED_RTOL iterations 1
1 SNES Function norm 4.144493702305e-02
Linear solve converged due to CONVERGED_RTOL iterations 1
2 SNES Function norm 6.309075568032e-03
Linear solve converged due to CONVERGED_RTOL iterations 1
3 SNES Function norm 3.359792279909e-04
Linear solve converged due to CONVERGED_RTOL iterations 1
4 SNES Function norm 1.198827244256e-06
Linear solve converged due to CONVERGED_RTOL iterations 1
5 SNES Function norm 1.545029314765e-11
```



Sample output (SNES and KSP)

```
SNES Object: 1 MPI processes
  type: ls
    line search variant: CUBIC
    alpha=1.000000000000e-04, maxstep=1.000000000000e+08, minlambd
    damping factor=1.000000000000e+00
  maximum iterations=50, maximum function evaluations=10000
  tolerances: relative=1e-08, absolute=1e-50, solution=1e-08
  total number of linear solver iterations=5
  total number of function evaluations=6
  KSP Object:   1 MPI processes
    type: gmres
      GMRES: restart=30, using Classical (unmodified) Gram-Schmidt
      GMRES: happy breakdown tolerance 1e-30
    maximum iterations=10000, initial guess is zero
    tolerances:  relative=1e-05, absolute=1e-50, divergence=10000
    left preconditioning
    using PRECONDITIONED norm type for convergence test
```

Sample output (PC and Mat)

```
PC Object:   1 MPI processes
  type: lu
    LU: out-of-place factorization
    tolerance for zero pivot 2.22045e-14
    matrix ordering: nd
    factor fill ratio given 5, needed 2.95217
      Factored matrix follows:
        Matrix Object:           1 MPI processes
          type: seqaij
          rows=100, cols=100
          package used to perform factorization: petsc
          total: nonzeros=1358, allocated nonzeros=1358
          total number of mallocs used during MatSetValues calls
            not using I-node routines
  linear system matrix = precond matrix:
  Matrix Object:     1 MPI processes
    type: seqaij
    rows=100, cols=100
    total: nonzeros=460, allocated nonzeros=460
    total number of mallocs used during MatSetValues calls =0
      not using I-node routines
```

In parallel

- `$ mpiexec -n 4 ./ex5 -da_grid_x 10 -da_grid_y 10 -par 6.7 -snes_monitor -{ksp,snes}_converged_reason -snes_view -sub_pc_type lu`
- How does the performance change as you
  - vary the number of processes (up to 32 or 64)?
  - increase the problem size?
  - try inexact subdomain solve?
  - try overlapping method: `-pc_type asm -pc_asm_overlap 2`
  - simulate a big machine: `-pc_asm_blocks 512`
  - change the Krylov method: `-ksp_type ibcgs`
  - use algebraic multigrid: `-pc_type hypre`
  - use smoothed aggregation multigrid: `-pc_type ml`

FEM Setup

```
./bin/pythonscripts/PetscGenerateFEMQuadrature.py
  2 2 2 1 laplacian
  2 1 1 1 gradient
  src/snes/examples/tutorials/ex62.h
```

Jacobi

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_gmres_restart 100 -ksp_rtol 1.0e-9
    -ksp_monitor_short
  -pc_type jacobi
```

Block diagonal

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type additive
  -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_pc_type jacobi
```

Block triangular

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type multiplicati
  -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_pc_type jacobi
```

Diagonal Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type diag
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Upper triangular Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type upper
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Lower triangular Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type lower
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

Full Schur complement

```
ex62
  -run_type full -bc_type dirichlet -show_solution 0
  -refinement_limit 0.00625 -interpolate 1
  -snes_monitor_short -snes_converged_reason
    -snes_view
  -ksp_type fgmres -ksp_gmres_restart 100
    -ksp_rtol 1.0e-9 -ksp_monitor_short
  -pc_type fieldsplit -pc_fieldsplit_type schur
    -pc_fieldsplit_schur_factorization_type full
  -fieldsplit_velocity_ksp_type gmres
    -fieldsplit_velocity_pc_type lu
  -fieldsplit_pressure_ksp_rtol 1e-10
    -fieldsplit_pressure_pc_type jacobi
```

User Projects

Create a new code based upon SNES Example 5.

1. Create a new directory
   - `mkdir -p /home/knepley/proj/newsim/src`
2. Copy the source
   - `cp ex5.c /home/knepley/proj/newsim/src`
   - Add `myStuff.c` and `myStuff2.F`
3. Create a PETSc makefile

```
bin/ex5:  src/ex5.o src/myStuff.o src/myStuff2.o
  ${CLINKER} -o $@ $^ ${PETSC_SNES_LIB}
include ${PETSC_DIR}/conf/variables
include ${PETSC_DIR}/conf/rules
```

To get the project ready-made

`hg clone http://petsc.cs.iit.edu/petsc/tutorials/SimpleTutorial newsim`