The Portable Extensible Toolkit for Scientific Computing

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PETSc Hands-On
13th Workshop on the DOE ACTS Collection
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We want to enable users to, assess solver performance, and optimize solvers for particular problems.
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Outline

1. Controlling the Solver
2. Where do I begin?
3. How do I improve?
4. Debugging
5. Examples
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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-`-sub_ksp_type bicg`
-`-fieldsplit_1_pc_type jacobi`
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
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A Krylov solver builds a small model of a linear operator $A$, using a subspace defined by

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

where $r$ is the initial residual.

The small system is solved directly, and the solution is projected back to the original space.
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The small system is solved directly, and the solution is projected back to the original space.
Where do I begin?

What Should I Know About Krylov Solvers?

- They can handle low-mode errors
- They need preconditioners
- They do a lot of inner products
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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Where do I begin?

What if LU fails?

LU will fail for

- Singular problems
- Saddle-point problems

For saddles use `PCFIELDSPLIT`

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

M. Knepley (UC)

PETSc

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What if LU fails?

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- Separately solves each field
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How do I improve?

Outline

1. Controlling the Solver
2. Where do I begin?
3. How do I improve?
   - Look at what you have
   - Back off in steps
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5. Examples
3. How do I improve?
   - Look at what you have
   - Back off in steps
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 refinement
  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**.
How do I improve?

What did the convergence look like?

Use \texttt{-snes\_monitor} and \texttt{-ksp\_monitor}, or \texttt{-log\_summary}:

\begin{verbatim}
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
\end{verbatim}
How do I improve?

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
0 KSP Residual norm 0.223226
  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`:

<table>
<thead>
<tr>
<th>Event</th>
<th>Count</th>
<th>Time (sec)</th>
<th>Flops</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Time Max Ratio</td>
<td>Flops Max Ratio</td>
<td>Mflop/s</td>
</tr>
<tr>
<td>KSPSetUp</td>
<td>12</td>
<td>3.6259e-03</td>
<td>1.0</td>
<td>0.00e+00 0.0</td>
</tr>
<tr>
<td>KSPSolve</td>
<td>3</td>
<td>4.8937e-01</td>
<td>1.0</td>
<td>8.93e+05 1.0</td>
</tr>
<tr>
<td>SNESSEsolve</td>
<td>1</td>
<td>4.9477e-01</td>
<td>1.0</td>
<td>9.22e+05 1.0</td>
</tr>
</tbody>
</table>
How do I improve?

Look at what you have

### Look at timing

Use `-log_summary`:

<table>
<thead>
<tr>
<th>Event</th>
<th>Time (sec)</th>
<th>Flops</th>
<th>---</th>
<th>Global</th>
<th>---</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Max</td>
<td>Ratio</td>
<td>Max</td>
<td>Ratio</td>
<td>%T</td>
<td>%f</td>
</tr>
<tr>
<td>VecMDot</td>
<td>1.8904e-03</td>
<td>1.0</td>
<td>2.49e+04</td>
<td>1.0</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>MatMult</td>
<td>2.1026e-03</td>
<td>1.0</td>
<td>2.65e+05</td>
<td>1.0</td>
<td>0</td>
<td>29</td>
</tr>
<tr>
<td>PCApply</td>
<td>4.6001e-01</td>
<td>1.0</td>
<td>7.78e+05</td>
<td>1.0</td>
<td>58</td>
<td>84</td>
</tr>
<tr>
<td>KSPSetUp</td>
<td>3.6259e-03</td>
<td>1.0</td>
<td>0.00e+00</td>
<td>0.0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>KSPSolve</td>
<td>4.8937e-01</td>
<td>1.0</td>
<td>8.93e+05</td>
<td>1.0</td>
<td>61</td>
<td>97</td>
</tr>
<tr>
<td>SNESsSolve</td>
<td>4.9477e-01</td>
<td>1.0</td>
<td>9.22e+05</td>
<td>1.0</td>
<td>62100</td>
<td>0</td>
</tr>
</tbody>
</table>

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

<table>
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Use `-log_summary_python` to get this information as a Python module
How do I improve?

- Look at what you have
- Back off in steps
Weaken the KSP

GMRES $\Rightarrow$ 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 $\Rightarrow$ 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 $\Rightarrow$ ILU
- `-pc_type 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
Separate solves for block operators
- Physical insight for subsystems
- Have optimal PCs for simpler equations
- Suboptions \texttt{fs_fieldsplit\_0}\_*

Flexibly combine subsolves
- Jacobi: \texttt{fs_pc_fieldsplit\_type = additive}
- Gauss-Siedel: \texttt{fs_pc_fieldsplit\_type = multiplicative}
- Schur complement: \texttt{fs_pc_fieldsplit\_type = schur}
Stokes example

The common block preconditioners for Stokes require only options:

The Stokes System

\[
\begin{pmatrix}
A & B \\
B^T & 0
\end{pmatrix}
\]
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`

The common block preconditioners for Stokes require only options:

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

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_fieldsplit_schur_factorization_type diag`


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`

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

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_fieldsplit_schur_factorization_type_type upper`

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_fieldsplit_schur_factorization_type upper`


The common block preconditioners for Stokes require only options:

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

\[
\begin{pmatrix}
    I & 0 \\
    B^T A^{-1} & I
\end{pmatrix}
\begin{pmatrix}
    \hat{A} & 0 \\
    0 & \hat{S}
\end{pmatrix}
\begin{pmatrix}
    I & A^{-1} B \\
    0 & I
\end{pmatrix}
\]
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
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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.
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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 4.14493702305e-02
Linear solve converged due to CONVERGED_RTOL iterations 1
2  SNES  Function norm 6.30907568032e-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
SNES Object: 1 MPI processes
  type: ls
    line search variant: CUBIC
    alpha=1.00000000000000e-04, maxstep=1.00000000000000e+08, minlambda=1.00000000000000e-12
    damping factor=1.00000000000000e+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
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 =0
    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 icgs
- 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 jacob
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 multiplicative
-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

```bash
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
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`