

Nested and Hierarchical Solvers in PETSc

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SIAM Computational Science & Engineering
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The PETSc Team



Bill Gropp



Barry Smith



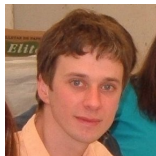
Satish Balay



Jed Brown



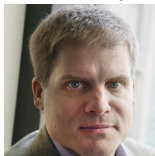
Matt Knepley



Lisandro Dalcin



Hong Zhang



Mark Adams



Peter Brune

The PETSc Team

IP8

THURS
1:00–1:45
Bill Gropp



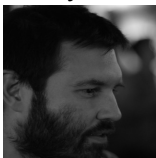
Barry Smith



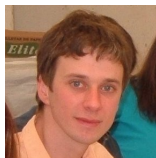
Satish Balay

MS186

THURS
10:00–10:25
Jed Brown



Matt Knepley



Lisandro Dalcin



Hong Zhang

MS87

TUES
3:00–3:25
Mark Adams

MS255

FRI
2:30–2:55
Peter Brune

Outline

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
```

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

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
```

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

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

Run flexible GMRES with 5 levels of multigrid as the preconditioner

```
./ex55 -ksp_type fgmres -pc_type mg -pc_mg_levels 5  
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Programming with Options

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```

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

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

```
-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
```

User Solve

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

```
SNESCreate(comm, &snest);  
SNESSetDM(snest, dm);  
SNESSetFromOptions(snest);  
DMCreateGlobalVector(dm, &u);  
SNESolve(snest, NULL, u);
```

Outline

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** **SNES** preconditions **SNES**

```
-ksp_type gmres
```

```
-snes_type ngmres
```

```
-pc_type richardson
```

```
-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
```


Outline

Why Can We Do This?

DM object handles

- discretization, and
- assembly

DM talks to solver through simple algebraic interface

- **IS**, list of integers
- Map between local and global spaces
- Maps between total and field spaces

DM Interface to Solver

Layout

- `DMGetLocalVector()`
- `DMGetGlobalVector()`
- `DMLocalToGlobalBegin()`, `DMLocalToGlobalEnd()`
- `DMGlobalToLocalBegin()`, `DMGlobalToLocalEnd()`

 S_L

DM Interface to Solver

Layout

- `DMGetLocalVector()`
- `DMGetGlobalVector()`
- `DMLocalToGlobalBegin()`, `DMLocalToGlobalEnd()`
- `DMGlobalToLocalBegin()`, `DMGlobalToLocalEnd()`

 S_L S

DM Interface to Solver

Layout

- `DMGetLocalVector()`
- `DMGetGlobalVector()`
- `DMLocalToGlobalBegin(), DMLocalToGlobalEnd()`
- `DMGlobalToLocalBegin(), DMGlobalToLocalEnd()`

$$S_L \longrightarrow S$$

DM Interface to Solver

Layout

- `DMGetLocalVector()`
- `DMGetGlobalVector()`
- `DMLocalToGlobalBegin()`, `DMLocalToGlobalEnd()`
- `DMGlobalToLocalBegin()`, `DMGlobalToLocalEnd()`

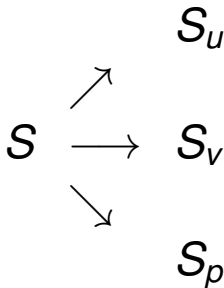
$$S_L \longleftrightarrow S$$

DM Interface to Solver

Field division

- `DMCreateFieldDecomposition()`
- `DMCreateSubDM()`
- `PCFieldSplitSetIS()`

Provides IS to Solver

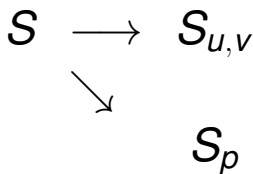


DM Interface to Solver

Field division

- `DMCreateFieldDecomposition()`
- `DMCreateSubDM()`
- `PCFieldSplitSetIS()`

Enables grouping of fields



DM Interface to Solver

Field division

- `DMCreateFieldDecomposition()`
- `DMCreateSubDM()`
- `PCFieldSplitSetIS()`

Need not use a DM

`(-pc_fieldsplit_detect_saddle_point)`

DM Interface to Solver

Multigrid

- `DMRefine()`, `DMCoarsen()`
- `DMCreateInterpolation()`
- `DMCreateInjection()`

Manages field map between levels

$$\begin{array}{ccc} S_u^H & \longleftrightarrow & S_u^h \\ S_v^H & \longleftrightarrow & S_v^h \\ S_p^H & \longleftrightarrow & S_p^h \end{array}$$

DM Interface to Solver

Multigrid

- `DMRefine()`, `DMCoarsen()`
- `DMCreateInterpolation()`
- `DMCreateInjection()`

Creates algebraic maps between spaces

$$S^H \longleftrightarrow S^h$$

DM Interface to Solver

Multigrid

- `DMRefine()`, `DMCoarsen()`
- `DMCreateInterpolation()`
- `DMCreateInjection()`

Optimization for residual interpolation

What Is Missing?

- NASM for unstructured grids (**DMPLex**)
- Nonlinear FieldSplit
- Combination of AMG-GMG
- Interface to modeling language (**UFL**)