

Nested and Hierarchical Solvers in PETSc

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SIAM Computational Science & Engineering
Boston, MA February 27, 2013



The PETSc Team



Matt Knepley



Barry Smith



Satish Balay



Jed Brown



Hong Zhang



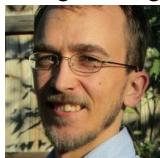
Lisandro Dalcin



Stefano Zampini



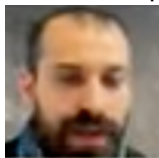
Mark Adams



Toby Issac



Hong Zhang



Pierre Jolivet



Junchao Zhang

The PETSc Team

IP8

THURS
1:00–1:45
Bill Gropp



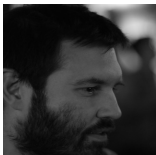
Barry Smith



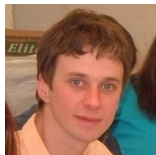
Satish Balay

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

- 1 Linear Examples
- 2 Nonlinear Examples
- 3 Design

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 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), Cohouet & Chabard, *IJNMF*, 1988.

```
-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), Elman, DTIC, 1994.

```
-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), Elman, DTIC, 1994.

```
-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, 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 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, 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 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, 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 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 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 jac  
-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 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, 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 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, 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
```

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

Solver Configuration: No New Code

ex31: P_2/P_1 Stokes Problem with Temperature on Unstructured Mesh

Additive Schwarz + Full Schur Complement, 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
```

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

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

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./ex55 -ksp_type fgmres -pc_type mg -pc_mg_levels 5  
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```

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-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, &snes);
```

```
SNESSetDM(snes, dm);
```

```
SNESSetFromOptions(snes);
```

```
DMCreateGlobalVector(dm, &u);
```

```
SNESolve(snes, NULL, u);
```

Outline

- 1 Linear Examples
- 2 Nonlinear Examples**
- 3 Design

Nonlinear Preconditioning

PC preconditions **KSP**

```
-ksp_type gmres
```

```
-pc_type richardson
```

SNES preconditions **SNES**

```
-snes_type ngmres
```

```
-npc_snes_type nrichardson
```

Nonlinear Preconditioning

PC preconditioners **KSP** **SNES** preconditioners **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

- 1 Linear Examples
- 2 Nonlinear Examples
- 3 Design**

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()`

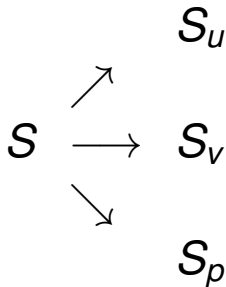
$$S_L \longleftrightarrow S$$

DM Interface to Solver

Field division

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

Provides IS to Solver

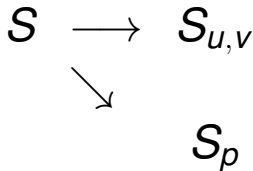


DM Interface to Solver

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**)