

Runtime Configurability in PETSc

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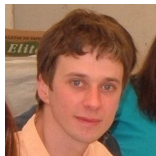
Satish Balay



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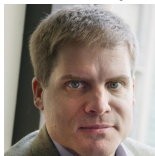
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What can be Configured in PETSc?

- Object behavior
 - Tolerances, subspace sizes, preallocation, ...
 - Eisenstat-Walker tolerances for **SNES**
- Concrete object types
 - **MATAIJ**, **KSPGMRES**, **SNESFAS**, **DMPLEX**
 - User-defined types
- Object organization
 - Linear & Nonlinear preconditioners
 - Number of splits in block methods
 - Explicit/Semi-implicit/Implicit division for **TS**

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Why Configure at Runtime?

Vectors and Matrices

- architecture
- problem/discretization

Solvers

- the equation and boundary conditions
- domain
- discretization
- solution evolution
 - nonlinear feedback
 - dynamic instabilities
 - strong or emergent anisotropy
 - resonance

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Why Configure at Runtime?

Arguments against concrete types in applications:

Programming Languages for Scientific Computing

Encyclopedia of Applied and Computational
Mathematics, Springer, 2012.

<http://arxiv.org/abs/1209.1711>

Outline

- 1 Configuring PETSc
- 2 Extending PETSc

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);
```

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
```

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 iterations C
```

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  
...
```

Nonlinear Preconditioning

Also called *globalization*

```
./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  
:  
21 SNES Function norm 585.143  
22 SNES Function norm 585.142  
23 SNES Function norm 585.142  
24 SNES Function norm 585.142  
:  
:
```

Nonlinear Preconditioning

Also called *globalization*

```
./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
```

```
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  
Nonlinear solve did not converge due to DIVERGED_INNER iterations 4
```

Nonlinear Preconditioning

Also called *globalization*

```
./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_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 42
Nonlinear solve did not converge due to DIVERGED_INNER iterations 4
```

Nonlinear Preconditioning

Also called *globalization*

```
./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

Also called *globalization*

```
./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 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 solve converged due to CONVERGED_FNORM_RELATIVE its 6
1 SNES Function norm 552.271
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 27
2 SNES Function norm 173.45
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 45
:
43 SNES Function norm 3.45407e-05
  Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
44 SNES Function norm 1.6141e-05
  Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
45 SNES Function norm 9.13386e-06
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 45
```

Nonlinear Preconditioning

Also called *globalization*

```
./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 solve converged due to CONVERGED_FNORM_RELATIVE its 6
1 SNES Function norm 538.605
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 13
2 SNES Function norm 178.005
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 24
:
27 SNES Function norm 0.000102487
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE its 2
28 SNES Function norm 4.2744e-05
  Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 2
29 SNES Function norm 1.01621e-05
  Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 29
```


Nonlinear Preconditioning

Also called *globalization*

```
./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_linesearch_type basic
-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 solve did not converge due to DIVERGED_MAX_IT its 6
  :
  Nonlinear solve converged due to CONVERGED_SNORM_RELATIVE its 1
  :
1 SNES Function norm 0.1935
2 SNES Function norm 0.0179938
3 SNES Function norm 0.00223698
4 SNES Function norm 0.000190461
5 SNES Function norm 1.6946e-06
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 5
```

Nonlinear Preconditioning

Also called *globalization*

```
./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 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 541.462
```

```
2 SNES Function norm 162.92
```

```
3 SNES Function norm 48.8138
```

```
4 SNES Function norm 11.1822
```

```
5 SNES Function norm 0.181469
```

```
6 SNES Function norm 0.00170909
```

```
7 SNES Function norm 3.24991e-08
```

```
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 7
```

Nonlinear Preconditioning

Also called *globalization*

```
./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 544.404
```

```
2 SNES Function norm 18.2513
```

```
3 SNES Function norm 0.488689
```

```
4 SNES Function norm 0.000108712
```

```
5 SNES Function norm 5.68497e-08
```

```
Nonlinear solve converged due to CONVERGED_FNORM_RELATIVE iterations 5
```

Nonlinear Preconditioning

Also called *globalization*

See discussion in:

Composing scalable nonlinear solvers,

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

ANL/MCS-P2010-0112, Argonne National Laboratory, 2012.

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

Outline

1 Configuring PETSc

2 Extending PETSc

- Creating a new Class Implementation
- Distributing your new Implementation

Outline

- 2 Extending PETSc
 - Creating a new Class Implementation
 - Distributing your new Implementation

Creating a Preconditioner (**PC**)

Include the private header for access to the **PC** struct:

```
#include<petsc-private/pcimpl.h>
```

Creating a Preconditioner (PC)

Define a struct for the concrete type:

```
typedef struct {  
    /* The maximum and actual half-bandwidth */  
    PetscInt   kmax, k;  
    /* The limit and actual norm fraction */  
    PetscReal frac, f;  
    /* The banded approximation */  
    Mat B;  
    /* The embedded PC */  
    PC pc;  
} PC_Banded;
```


Creating a Preconditioner (PC)

Register a constructor for the concrete type:

```
PCRegister("banded", PCCreate_Banded)
```

Creating a Preconditioner (PC)

Define the constructor:

```
PetscErrorCode PCCreate_Banded(PC pc)
{
    PC_Banded      *b;
    PetscErrorCode ierr;

    PetscFunctionBegin;
    /* Create concrete type struct */
    /* Setup function table for class */
    /* Setup concrete type-specific functions */
    /* Setup subobjects */
    PetscFunctionReturn(0);
}
```

Creating a Preconditioner (PC)

Define the constructor:

```
PetscErrorCode PCCreate_Banded(PC pc)
{
    PetscFunctionBegin;
    ierr = PetscNewLog(pc, &b);CHKERRQ(ierr);
    pc->data = (void *) b;
    b->kmax = 50;
    b->frac = 0.95;
    /* Setup function table for class */
    /* Setup concrete type-specific functions */
    /* Setup subobjects */
    PetscFunctionReturn(0);
}
```

Creating a Preconditioner (PC)

Define the constructor:

```
PetscErrorCode PCCreate_Banded(PC pc)
{
    PetscFunctionBegin;
    /* Create concrete type struct */
    pc->ops->apply                = PCApply_Banded;
    pc->ops->applytranspose        = NULL;
    pc->ops->setup                 = PCSetUp_Banded;
    pc->ops->reset                 = PCReset_Banded;
    pc->ops->destroy               = PCDestroy_Banded;
    pc->ops->setfromoptions        = PCSetFromOptions_Banded;
    pc->ops->view                  = PCView_Banded;
    pc->ops->applyrichardson       = NULL;
    pc->ops->appliesymmetricleft   = NULL;
    pc->ops->appliesymmetricright = NULL;
    /* Setup concrete type-specific functions */
    /* Setup subobjects */
    PetscFunctionReturn(0);
}
```

Creating a Preconditioner (PC)

Define the constructor:

```
PetscErrorCode PCCreate_Banded(PC pc)
{
    PetscFunctionBegin;
    /* Create concrete type struct */
    /* Setup function table for class */
    PetscObjectComposeFunction((PetscObject) pc,
        "PCBandedSetMaxHalfBandwidth_C", PCBandedSetMaxHalfBandwidth_Banded);
    PetscObjectComposeFunction((PetscObject) pc,
        "PCBandedSetNormFraction_C", PCBandedSetNormFraction_Banded);
    /* Setup subobjects */
    PetscFunctionReturn(0);
}
```

Creating a Preconditioner (PC)

Define the constructor:

```
PetscErrorCode PCCreate_Banded(PC pc)
{
    PetscFunctionBegin;
    /* Create concrete type struct */
    /* Setup function table for class */
    /* Setup concrete type-specific functions */
    {
        const char *prefix;

        PCCreate(PetscObjectComm((PetscObject) pc), &b->pc);
        PetscObjectGetOptionsPrefix((PetscObject) pc, &prefix);
        PetscObjectSetOptionsPrefix((PetscObject) b->pc, prefix);
        PetscObjectAppendOptionsPrefix((PetscObject) b->pc, "banded_");
    }
    PetscFunctionReturn(0);
}
```

Creating a Preconditioner (PC)

Define concrete type-specific functions:

```
PetscErrorCode PCBandedSetMaxHalfBandwidth(PC pc, PetscInt kmax)
{
    PetscErrorCode ierr;

    PetscFunctionBegin;
    PetscValidHeaderSpecific(pc, PC_CLASSID, 1);
    PetscTryMethod(pc, "PCBandedSetMaxHalfBandwidth_C",
        (PC, PetscInt), (pc, kmax));
    PetscFunctionReturn(0);
}
```

Outline

- 2 Extending PETSc
 - Creating a new Class Implementation
 - Distributing your new Implementation

Distributing a Shared Library

Package Initialization

- Register classes,
- concrete type constructors,
- logging events,
- and finalizer with

```
PetscRegisterFinalize()
```

Distributing a Shared Library

Package Finalization

- Destroy list of constructors,
- and class memory allocations

Distributing a Shared Library

Package Loading

- Library located using

```
-dll_append/prepend <libname>
```

- PETSc calls

```
PetscDLLLibraryRegister_<libname>()
```

- No recompiling or relinking of PETSc libraries or user code