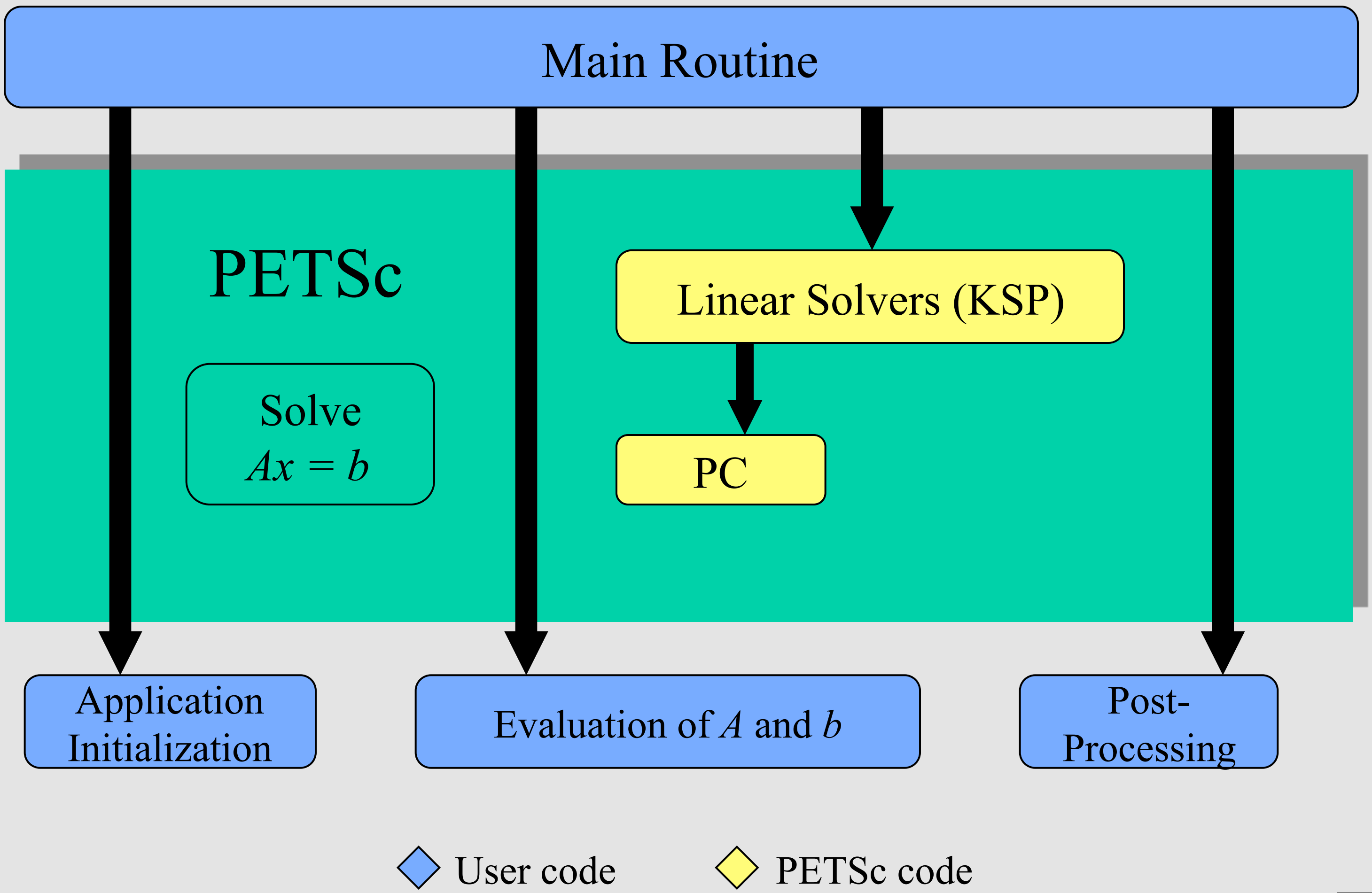
Introduction to PETSc
KSP, PC

CS595, Fall 2010

Linear Solution



beginner

solvers: linear

Creating the KSP Context

- C/C++ version

```
ierr = KSPCreate(PETSC_COMM_WORLD,  &ksp);
```

- Fortran version

```
call  KSPCreate(PETSC_COMM_WORLD,  ksp,  ierr)
```

- Provides an **identical** user interface for all linear solvers
  - uniprocess and parallel
  - real and complex numbers

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Context Variables

- Are the key to solver organization
- Contain the complete state of an algorithm, including
  - parameters (e.g., convergence tolerance)
  - functions that run the algorithm (e.g., convergence monitoring routine)
  - information about the current state (e.g., iteration number)

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KSP Structure

- Each KSP object actually contains two parts:
  - Krylov Space Method
    - The iterative method
    - The context contains information on method parameters (e.g., GMRES search directions), work spaces, etc
  - PC — Preconditioners
    - Knows how to apply a preconditioner
    - The context contains information on the preconditioner, such as what routine to call to apply it

Linear Solvers in PETSc

Krylov Methods (KSP)

- Conjugate Gradient
- GMRES
- CG-Squared
- Bi-CG-stab
- Transpose-free QMR
- etc.

Preconditioners (PC)

- Block Jacobi
- Overlapping Additive Schwarz
- ICC, ILU (sequential only)
- ILU(k), LU (direct solve, sequential only)
- Arbitrary matrix
- etc.

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Basic Linear Solver Code (C/C++)

```
KSP    ksp;          /*  linear solver context  */
Mat    A;            /*  matrix  */
Vec    x, b;         /*  solution, RHS vectors  */
int    n, its;       /*  problem dimension, number of iterations  */

MatCreate(PETSC_COMM_WORLD,PETSC_DECIDE,PETSC_DECIDE,n,n,&A);
MatSetFromOptions(A);
/* (code to assemble matrix not shown) */
VecCreate(PETSC_COMM_WORLD,&x);
VecSetSizes(x,PETSC_DECIDE, n);
VecSetFromOptions(x);
VecDuplicate(x,&b);
/* (code to assemble RHS vector not shown)*/

KSPCreate(PETSC_COMM_WORLD, &ksp);
KSPSetOperators(ksp, A, A, DIFFERENT_NONZERO_PATTERN);
KSPSetFromOptions(ksp);
KSPSolve(ksp, b, x);
KSPDestroy(ksp);
```

Indicate whether the preconditioner has the same nonzero pattern as the matrix *each time a system is solved.* This default works with *all* preconditioners. Other values (e.g., SAME_NONZERO_PATTERN) can be used for particular preconditioners. Ignored when solving only one system

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Basic Linear Solver Code (Fortran)

```
KPS       ksp
Mat       A
Vec       x, b
integer   n, its, ierr

call  MatCreate( PETSC_COMM_WORLD,PETSC_DECIDE,n,n,A,ierr )
call  MatSetFromOptions( A, ierr )
call  VecCreate( PETSC_COMM_WORLD,x,ierr )
call  VecSetSizes( x, PETSC_DECIDE, n, ierr )
call  VecSetFromOptions( x, ierr )
call  VecDuplicate( x,b,ierr )

          C     then assemble matrix and right-hand-side vector

call  KSPCreate(PETSC_COMM_WORLD,ksp,ierr)
call  KSPSetOperators(ksp,A,A,DIFFERENT_NONZERO_PATTERN,ierr)
call  KSPSetFromOptions(ksp,ierr)
call  KSPSolve(ksp,b,x,ierr)
call  KSPDestroy(ksp,ierr)
```

Customization Options

- Command Line Interface
  - Applies same rule to all queries via a database
  - Enables the user to have complete control at runtime, with no extra coding
- Procedural Interface
  - Provides a great deal of control on a usage-by-usage basis inside a single code
  - Gives full flexibility inside an application

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Setting Solver Options at Runtime

- -ksp_type [cg, gmres, bcgs, tfqmr,…]
- -pc_type [lu, ilu, jacobi, sor, asm,…]

1

2

- -ksp_max_it <max_iters>
- -ksp_gmres_restart <restart>
- -pc_asm_overlap <overlap>
- -pc_asm_type [basic, restrict, interpolate, none]
- etc ...

1 beginner | 2 intermediate

solvers: linear

Linear Solvers: Monitoring Convergence

- -ksp_monitor - Monitor preconditioned residual norm
- -ksp_monitor_solution - Monitor solution graphically

1

- -ksp_monitor_true_residual - Monitor true residual norm || b-Ax ||
- -ksp_monitor_singular_value - Monitor singular values

2

- User-defined monitors, using callbacks

3

1	2	3
beginner	intermediate	advanced

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Setting Solver Options within Code

  - KSPSetType(KSP ksp,KSPType type)
  - KSPSetTolerances(KSP ksp,PetscReal rtol, PetscReal atol,PetscReal dtol, int maxits)
  - etc....
- KSPGetPC(KSP ksp,PC *pc)
  - PCSetType(PC pc,PCType)
  - PCASMSetOverlap(PC pc,int overlap)
  - etc....

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Recursion: Specifying Solvers for Schwarz Preconditioner Blocks

- Specify KSP solvers and options with "-sub" prefix, e.g.,
  - Full or incomplete factorization

    -sub_pc_type lu

    -sub_pc_type ilu -sub_pc_ilu_levels <levels>
  - Can also use inner Krylov iterations, e.g.,

    -sub_ksp_type gmres -sub_ksp_rtol <rtol>

    -sub_ksp_max_it <maxit>

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solvers: linear: preconditioners

KSP: Review of Basic Usage

- KSPCreate( ) - Create solver context
- KSPSetOperators( ) - Set linear operators
- KSPSetFromOptions( ) - Set runtime solver options for [KSP,PC]
- KSPSolve( ) - Run linear solver
- KSPView( ) - View solver options actually used at runtime (alternative: -ksp_view)
- KSPDestroy( ) - Destroy solver

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KSP: Review of Selected Preconditioner Options

Functionality	Procedural Interface	Runtime Option	
Set preconditioner type	PCSetType( )	-pc_type [lu,ilu,jacobi, sor,asm,…]	1
Set level of fill for ILU	PCILUSetLevels( )	-pc_ilu_levels <levels>	2
Set SOR iterations	PCSORSetIterations( )	-pc_sor_its <its>	
Set SOR parameter	PCSORSetOmega( )	-pc_sor_omega <omega>	
Set additive Schwarz variant	PCASMSetType( )	-pc_asm_type [basic, restrict,interpolate,none]	
Set subdomain solver options	PCGetSubKSP( )	-sub_pc_type <pctype> -sub_ksp_type <ksptype> -sub_ksp_rtol <rtol>	

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And many more options...

solvers: linear: preconditioners

Review of Selected Krylov Method Options

Functionality	Procedural Interface	Runtime Option
Set Krylov method	KSPSetType( )	-ksp_type [cg,gmres,bcgs, tfqmr,cgs,…] (1)
Set monitoring routine	KSPSetMonitor( )	-ksp_monitor, -ksp_monitor_true_residual, -ksp_singular_value
Set convergence tolerances	KSPSetTolerances( )	-ksp_rtol <rt> -ksp_atol <at> -ksp_max_its <its> (2)
Set GMRES restart parameter	KSPGMRESSetRestart( )	-ksp_gmres_restart <restart>
Set orthogonalization routine for GMRES	KSPGMRESSetOrthogonalization( )	-ksp_gmres_classicalgramschmidt -ksp_gmres_modifiedgramschmidt

And many more options...

1 beginner | 2 intermediate

solvers: linear: Krylov methods

Why Polymorphism?

- Programs become independent of the choice of algorithm
- Consider the question:
  - What is the best combination of iterative method and preconditioner for my problem?
- How can you answer this experimentally?
  - Old way:
    - Edit code. Make. Run. Edit code. Make. Run. Debug. Edit. …
  - New way:…

KSP: Runtime Script Example

emacs@lava.mcs.anl.gov

Buffers Files Tools Edit Search Insert Help

```
#! /bin/csh
#
# Sample script: Experimenting with linear solver options.
# Can be used with, e.g., petsc/src/sles/examples/tutorials/ex2.c
#
foreach np (1 2 4 8)                          # number of processors
  foreach ksptype (gmres bcgs tfqmr)          # Krylov solver
    foreach pctype (bjacobi asm)              # preconditioner
      foreach subpctype (jacobi sor ilu)      # subdomain solver
        if ($subpctype == ilu) then
          foreach level (0 1 2)               # level of fill for ILU(k)
          echo '****** Beginning new run ******'
            mpirun -np $np ex2 -pc_type $pctype -ksp_type $ksptype \
               -sub_ksp_type preonly sub_pc_type $subpctype \
               -sub_pc_ilu_levels $level \
                -ksp_monitor -sles_view -optionsleft
        else
          echo '****** Beginning new run ******'
          mpirun -np $np ex2 -pc_type $pctype -ksp_type $ksptype \
               -sub_ksp_type preonly sub_pc_type $subpctype \
                -ksp_monitor -sles_view -optionsleft
        endif
      end
    end
  end
end
-----Emacs: script1            (Shell-script)--L1--Top----------------
```

intermediate

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Viewing KSP Runtime Options

```
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Buffers Files Tools Edit Search Help
[lava] ex2 -ksp_monitor -pc_ilu_levels 1 -sles_view > out.5
0 KSP Residual norm 5.394188560416e+00
1 KSP Residual norm 1.238309089931e+00
2 KSP Residual norm 1.104133215450e-01
3 KSP Residual norm 6.609740098311e-03
4 KSP Residual norm 2.732911209560e-04
KSP Object:
  method: gmres
    GMRES: restart=30, using Modified Gram-Schmidt Orthogonalization
  maximum iterations=10000, initial guess is zero
  tolerances:  relative=0.000138889, absolute=1e-50, divergence=10000
  left preconditioning
PC Object:
  method: ilu
    ILU: 1 level of fill
         out-of-place factorization
         matrix ordering: natural
  linear system matrix = precond matrix:
Matrix Object:
  type=MATSEQAIJ, rows=56, cols=56
  total: nonzeros=250, allocated nonzeros=560
Norm of error 0.000280658 iterations 4

-----Emacs: out.5              (Nroff)--L1--All------------------------
```

intermediate

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Providing Different Matrices to Define Linear System and Preconditioner

Solve $Ax=b$

Precondition via: $M_L^{-1} A M_R^{-1} (M_R x) = M_L^{-1} b$

- Krylov method: Use A for matrix-vector products
- Build preconditioner using either
  - A - matrix that defines linear system
  - or P - a different matrix (cheaper to assemble)
- KSPSetOperators(KSP ksp,
  - Mat A,
  - Mat P,
  - MatStructure flag)

advanced

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Matrix-Free Solvers

- Use "shell" matrix data structure
  - MatCreateShell(…, Mat *mfctx)
- Define operations for use by Krylov methods
  - MatShellSetOperation(Mat mfctx,
    - MatOperation MATOP_MULT,
    - (void *) int (UserMult)(Mat, Vec, Vec))
- Names of matrix operations defined in

  petsc/include/petscmat.h
- Some defaults provided for nonlinear solver usage

advanced

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