PETSc Tutorial
Numerical Software Libraries for the Scalable Solution of PDEs

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http://www.mcs.anl.gov/petsc

Intended for use with version 2.1.0 of PETSc

Tutorial Objectives

• Introduce the Portable, Extensible Toolkit for Scientific Computation (PETSc)
• Demonstrate how to write a complete parallel implicit PDE solver using PETSc
• Introduce PETSc interfaces to other software packages
• Explain how to learn more about PETSc
The Role of PETSc

- Developing parallel, non-trivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.
- PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver nor a silver bullet.

What is PETSc?

- A freely available and supported research code
  - Available via http://www.mcs.anl.gov/petsc
  - Free for everyone, including industrial users
  - Hyperlinked documentation and manual pages for all routines
  - Many tutorial-style examples
  - Support via email: petsc-maint@mcs.anl.gov
  - Usable from Fortran 77/90, C, and C++
- Portable to any parallel system supporting MPI, including
  - Tightly coupled systems
    - Cray T3E, SGI Origin, IBM SP, HP 9000, Sun Enterprise
  - Loosely coupled systems, e.g., networks of workstations
    - Compaq, HP, IBM, SGI, Sun
    - PCs running Linux or Windows
- PETSc history
  - Begun in September 1991
  - Now: over 8,500 downloads since 1995 (versions 2.0 and 2.1)
- PETSc funding and support
  - Department of Energy: MICS Program, DOE2000, SciDAC
  - National Science Foundation, Multidisciplinary Challenge Program, CISE
PETSc Concepts

- How to specify the mathematics of the problem
  - Data objects
    - vectors, matrices

- How to solve the problem
  - Solvers
    - linear, nonlinear, and time stepping (ODE) solvers

- Parallel computing complications
  - Parallel data layout
    - structured and unstructured meshes

Tutorial Approach

From the perspective of an application programmer:

<table>
<thead>
<tr>
<th>Beginner</th>
<th>Advanced</th>
</tr>
</thead>
<tbody>
<tr>
<td>basic functionality, intended for use by most programmers</td>
<td>user-defined customization of algorithms and data structures</td>
</tr>
</tbody>
</table>

**Emphasis of this tutorial**

<table>
<thead>
<tr>
<th>Intermediate</th>
<th>Developer</th>
</tr>
</thead>
<tbody>
<tr>
<td>selecting options, performance evaluation and tuning</td>
<td>advanced customizations, intended primarily for use by library developers</td>
</tr>
</tbody>
</table>

- beginner
- intermediate
- advanced
- developer
Structure of PETSc

PETSc PDE Application Codes
- ODE Integrators
- Visualization
- Nonlinear Solvers, Unconstrained Minimization
- Grid Management
- Linear Solvers
- Preconditioners + Krylov Methods
- Profiling Interface
- PETSc PDE Application Codes
- MPI, MPI-IO, BLAS, LAPACK

Computation and Communication Kernels
- PETSc PDE Application Codes
- Object-Oriented
- Matrices, Vectors, Indices
- Profiling Interface
- Computation and Communication Kernels
- MPI, MPI-IO, BLAS, LAPACK

Compressed Sparse Row (AIJ)
- Blocked Compressed Sparse Row (BAIJ)
- Block Diagonal (BDIAG)
- Dense
- Matrix-free
- Other

Distributed Arrays
- Matrices
- Index Sets
- Vectors

PETSc Numerical Components

Nonlinear Solvers
- Newton-based Methods
- Line Search
- Trust Region
- Other

Time Steppers
- Euler
- Backward Euler
- Pseudo Time Stepping
- Other

Krylov Subspace Methods
- GMRES
- CG
- CGS
- Bi-CG-STAB
- TFQMR
- Richardson
- Chebychev
- Other

Preconditioners
- Additive Schwartz
- Block Jacobi
- Jacobi
- ILU
- ICC (Sequential only)
- LU
- Others

Matrices

Index Sets
- Indices
- Block Indices
- Stride
- Other

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ACTS Toolkit Workshop
What is not in PETSc?

- Discretizations
- Unstructured mesh generation and refinement tools
- Load balancing tools
- Sophisticated visualization capabilities

But PETSc does interface to external software that provides some of this functionality.

Solver Definitions: For Our Purposes

- **Explicit**: Field variables are updated using neighbor information (no global linear or nonlinear solves)
- **Semi-implicit**: Some subsets of variables (e.g., pressure) are updated with global solves
- **Implicit**: Most or all variables are updated in a single global linear or nonlinear solve
Focus On Implicit Methods

• Explicit and semi-explicit are easier cases
• No direct PETSc support for
  – ADI-type schemes
  – spectral methods
  – particle-type methods

Numerical Methods Paradigm

• Encapsulate the latest numerical algorithms in a consistent, application-friendly manner
• Use mathematical and algorithmic objects, not low-level programming language objects
• Application code focuses on mathematics of the global problem, not parallel programming details
PETSc Programming Aids

- Correctness Debugging
  - Automatic generation of tracebacks
  - Detecting memory corruption and leaks
  - Optional user-defined error handlers
- Performance Debugging
  - Integrated profiling using -log_summary
  - Profiling by stages of an application
  - User-defined events

The PETSc Programming Model

- Goals
  - Portable, runs everywhere
  - Performance
  - Scalable parallelism
- Approach
  - Distributed memory, “shared-nothing”
    - Requires only a compiler (single node or processor)
    - Access to data on remote machines through MPI
  - Can still exploit “compiler discovered” parallelism on each node (e.g., SMP)
  - Hide within parallel objects the details of the communication
  - User orchestrates communication at a higher abstract level than message passing
Collectivity

- MPI communicators (MPI_Comm) specify collectivity (processors involved in a computation)
- All PETSc creation routines for solver and data objects are collective with respect to a communicator, e.g.,
  - VecCreate(MPI_Comm comm, int m, int M, Vec *x)
- Some operations are collective, while others are not, e.g.,
  - collective: VecNorm()
  - not collective: VecGetLocalSize()
- If a sequence of collective routines is used, they must be called in the same order on each processor.

Hello World

```c
#include "petsc.h"
int main( int argc, char *argv[] )
{
  PetscInitialize(&argc,&argv,PETSC_NULL,PETSC_NULL);
  PetscPrint(PETSC_COMM_WORLD,"Hello World\n");
  PetscFinalize();
  return 0;
}
```
Data Objects

- Vectors (Vec)
  - focus: field data arising in nonlinear PDEs
- Matrices (Mat)
  - focus: linear operators arising in nonlinear PDEs (i.e., Jacobians)

- Object creation
- Object assembly
- Setting options
- Viewing
- User-defined customizations

Vectors

- What are PETSc vectors?
  - Fundamental objects for storing field solutions, right-hand sides, etc.
  - Each process locally owns a subvector of contiguously numbered global indices
- Create vectors via
  - VecCreate(...,Vec *)
    - MPI_Comm - processors that share the vector
    - number of elements local to this processor
    - or total number of elements
  - VecSetType(Vec,VecType)
    - Where VecType is
      - VEC_SEQ, VEC_MPI, or VEC_SHARED
Vector Assembly

- VecSetValues(Vec,...)
  - number of entries to insert/add
  - indices of entries
  - values to add
  - mode: [INSERT_VALUES,ADD_VALUES]
- VecAssemblyBegin(Vec)
- VecAssemblyEnd(Vec)

Parallel Matrix and Vector Assembly

- Processors may generate any entries in vectors and matrices
- Entries need not be generated on the processor on which they ultimately will be stored
- PETSc automatically moves data during the assembly process if necessary
Selected Vector Operations

<table>
<thead>
<tr>
<th>Function Name</th>
<th>Operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>VecAXPY(Scalar *a, Vec x, Vec y)</td>
<td>( y = y + a \times x )</td>
</tr>
<tr>
<td>VecAYPX(Scalar *a, Vec x, Vec y)</td>
<td>( y = x + a \times y )</td>
</tr>
<tr>
<td>VecWAXPY(Scalar *a, Vec x, Vec y, Vec w)</td>
<td>( w = a \times x + y )</td>
</tr>
<tr>
<td>VecScale(Scalar *a, Vec x)</td>
<td>( x = a \times x )</td>
</tr>
<tr>
<td>VecCopy(Vec x, Vec y)</td>
<td>( y = x )</td>
</tr>
<tr>
<td>VecPointwiseMult(Vec x, Vec y, Vec w)</td>
<td>( w_i = x_i \times y_i )</td>
</tr>
<tr>
<td>VecMax(Vec x, int *idx, double *r)</td>
<td>( r = \max x_i )</td>
</tr>
<tr>
<td>VecShift(Scalar *s, Vec x)</td>
<td>( x_i = s + x_i )</td>
</tr>
<tr>
<td>VecAbs(Vec x)</td>
<td>( x_i =</td>
</tr>
<tr>
<td>VecNorm(Vec x, NormType type, double *r)</td>
<td>( r = |x| )</td>
</tr>
</tbody>
</table>

Simple Example Programs

Location: petsc/src/sys/examples/tutorials/

- ex2.c - synchronized printing

Location: petsc/src/vec/examples/tutorials/

- ex1.c, ex1f.F, ex1f90.F - basic vector routines
- ex3.c, ex3f.F - parallel vector layout

And many more examples ...

- on-line exercise
Matrices

- What are PETSc matrices?
  - Fundamental objects for storing linear operators (e.g., Jacobians)
- Create matrices via
  - MatCreate(..., Mat *)
    - MPI_Comm - processors that share the matrix
    - number of local/global rows and columns
  - MatSetType(Mat, MatType)
    - where MatType is one of
      - default sparse AIJ: MPIAIJ, SEQAIJ
      - block sparse AIJ (for multi-component PDEs): MPIAIJ, SEQAIJ
      - symmetric block sparse AIJ: MPIISBAIJ, SAEGSBAIJ
      - block diagonal: MPIBDIAG, SEQBDIAG
      - dense: MPIDENSE, SEQDENSE
      - matrix-free
      - etc.

Matrices and Polymorphism

- Single user interface, e.g.,
  - Matrix assembly
    - MatSetValues()
  - Matrix-vector multiplication
    - MatMult()
  - Matrix viewing
    - MatView()
- Multiple underlying implementations
  - AIJ, block AIJ, symmetric block AIJ, block diagonal, dense, matrix-free, etc.
Matrix Assembly

- **MatSetValues(Mat, ...)**
  - number of rows to insert/add
  - indices of rows and columns
  - number of columns to insert/add
  - values to add
  - mode: [INSERT_VALUES, ADD_VALUES]
- **MatAssemblyBegin(Mat)**
- **MatAssemblyEnd(Mat)**

```c
Mat A;
int column[3], i, start, end;
double value[3];

/* mesh interior */
value[0] = -1.0; value[1] = 2.0; value[2] = -1.0;
for (i=start; i<end; i++) {
    column[0] = i-1; column[1] = i; column[2] = i+1;
    MatSetValues(A, 1, &i, 3, column, value, INSERT_VALUES);
}
/* also must set boundary points */
MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
```

Matrix Assembly Example

simple 3-point stencil for 1D discretization

```c
Mat A;
int column[3], i, start, end;
double value[3];

/* mesh interior */
value[0] = -1.0; value[1] = 2.0; value[2] = -1.0;
for (i=start; i<end; i++) {
    column[0] = i-1; column[1] = i; column[2] = i+1;
    MatSetValues(A, 1, &i, 3, column, value, INSERT_VALUES);
}
/* also must set boundary points */
MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
```
Parallel Matrix Distribution

Each process locally owns a submatrix of contiguously numbered global rows.

```
proc 0
proc 1
proc 2
proc 3
proc 4
} proc 3: locally owned rows
```

MatGetOwnershipRange(Mat A, int *rstart, int *rend)
- `rstart`: first locally owned row of global matrix
- `rend-1`: last locally owned row of global matrix

Viewers

- Printing information about solver and data objects
- Visualization of field and matrix data
- Binary output of vector and matrix data
Viewer Concepts

- Information about PETSc objects
  - runtime choices for solvers, nonzero info for matrices, etc.
- Data for later use in restarts or external tools
  - vector fields, matrix contents
  - various formats (ASCII, binary)
- Visualization
  - *simple* x-window graphics
    - vector fields
    - matrix sparsity structure

Viewing Vector Fields

- VecView(Vec x, PetscViewer v);
- Default viewers
  - ASCII (sequential):
    - PETSC_VIEWER_STDOUT_SELF
  - ASCII (parallel):
    - PETSC_VIEWER_STDOUT_WORLD
  - X-windows:
    - PETSC_VIEWER_DRAW_WORLD
- Default ASCII formats
  - PETSC_VIEWER_ASCII_DEFAULT
  - PETSC_VIEWER_ASCII_MATLAB
  - PETSC_VIEWER_ASCII_COMMON
  - PETSC_VIEWER_ASCII_INFO
  - etc.

Solution components, using runtime option \
-snes_vecmonitor

- velocity: $u$
- velocity: $v$
- vorticity: $\zeta$
- temperature: $T$
**Viewing Matrix Data**

- MatView(Mat A, PetscViewer v);
- Runtime options available after matrix assembly
  - -mat_view_info
    - info about matrix assembly
  - -mat_view_draw
    - sparsity structure
  - -mat_view
    - data in ASCII
  - etc.

**Solvers: Usage Concepts**

<table>
<thead>
<tr>
<th>Solver Classes</th>
<th>Usage Concepts</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear (SLES)</td>
<td>Context variables</td>
</tr>
<tr>
<td>Nonlinear (SNES)</td>
<td>Solver options</td>
</tr>
<tr>
<td>Timestepping (TS)</td>
<td>Callback routines</td>
</tr>
<tr>
<td></td>
<td>Customization</td>
</tr>
</tbody>
</table>

**important concepts**
Linear PDE Solution

Main Routine

PETSc

Solve $Ax = b$

Application Initialization

Evaluation of $A$ and $b$

Post-Processing

Linear Solvers (SLES)

PC

KSP

PETSc code

User code

Solvers:
linear

Nonlinear Solvers (SNES)

Timestepping Solvers (TS)

Linear Solvers (SLES)

PC

KSP

Application Initialization

Function Evaluation

Jacobian Evaluation

Post-Processing

SPA I

ILUDTP

Function Evaluation

Other Tools

PVODE

Other Tools

User code

PETSc code

PETSc

— PETSc Tutorial —
Linear Solvers

**Goal:** Support the solution of linear systems, 

\[ Ax = b, \]

particularly for sparse, parallel problems arising within PDE-based models

User provides:

- Code to evaluate \( A, b \)

---

Linear Solvers (SLES)

*SLES: Scalable Linear Equations Solvers*

- Application code interface
- Choosing the solver
- Setting algorithmic options
- Viewing the solver
- Determining and monitoring convergence
- Providing a different preconditioner matrix
- Matrix-free solvers
- User-defined customizations
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)

Creating the SLES Context

- C/C++ version
  ```c
  ierr = SLESCreate(MPI_COMM_WORLD,&sles);
  ```
- Fortran version
  ```fortran
  call SLESCreate(MPI_COMM_WORLD,sles,ierr)
  ```
- Provides an identical user interface for all linear solvers
  - uniprocessor and parallel
  - real and complex numbers
Linear Solvers in PETSc 2.0

Krylov Methods (KSP)
- Conjugate Gradient
- GMRES
- CG-Squared
- Bi-CG-stab
- Transpose-free QMR
- etc.

Preconditioners (PC)
- Block Jacobi
- Overlapping Additive Schwarz
- ICC, ILU via BlockSolve95
- ILU(k), LU (sequential only)
- etc.

Basic Linear Solver Code (C/C++)

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

MatCreate(MPI_COMM_WORLD,PETSC_DECIDE,PETSC_DECIDE,n,n,&A);    /* assemble matrix */
VecCreate(MPI_COMM_WORLD,PETSC_DECIDE,n,&x);                    /* assemble RHS vector */
VecDuplicate(x,&b);

SLESCreate(MPI_COMM_WORLD,&sles);
SLESSetOperators(sles,A,A,DIFFERENT_NONZERO_PATTERN);
SLESSetFromOptions(sles);
SLESSolve(sles,b,x,&its);
SLESDestroy(sles);
```

Customization Options

- Procedural Interface
  - Provides a great deal of control on a usage-by-usage basis inside a single code
  - Gives full flexibility inside an application
- 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

Setting Solver Options within Code

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

— skipped —
Recursion: Specifying Solvers for Schwarz Preconditioner Blocks

- Specify SLES 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>

Setting Solver Options at Runtime

- ksp_type [cg,gmres,bcgs,tfqmr,...]
- pc_type [lu,ilu,jacobi,sor,asm,...]
- ksp_max_it <max_iters>
- ksp_gmres_restart <restart>
- pc_asm_overlap <overlap>
- pc_asm_type [basic,restrict,interpolate,none]
- etc...

beginner  intermediate  solvers: linear: preconditioners

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ACTS Toolkit Workshop
Linear Solvers: Monitoring Convergence

- `-ksp_monitor` - Prints preconditioned residual norm
- `-ksp_xmonitor` - Plots preconditioned residual norm

- `-ksp_truemonitor` - Prints true residual norm \( \| b - Ax \| \)
- `-ksp_xtruemonitor` - Plots true residual norm \( \| b - Ax \| \)

- User-defined monitors, using callbacks

---

SLES: Review of Basic Usage

- `SLESCreate()` - Create SLES context
- `SLESSetOperators()` - Set linear operators
- `SLESSetFromOptions()` - Set runtime solver options for `[SLES, KSP, PC]`
- `SLESSolve()` - Run linear solver
- `SLESView()` - View solver options actually used at runtime (alternative: `-sles_view`)
- `SLESDestroy()` - Destroy solver
### SLES: Review of Selected Preconditioner Options

<table>
<thead>
<tr>
<th>Functionality</th>
<th>Procedural Interface</th>
<th>Runtime Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set preconditioner type</td>
<td>PCSetType()</td>
<td>-pc_type [lu,ilu,jacobi,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>sor,asm,...]</td>
</tr>
<tr>
<td>Set level of fill for ILU</td>
<td>PCILUSetLevels()</td>
<td>-pc_ilu_levels &lt;levels&gt;</td>
</tr>
<tr>
<td>Set SOR iterations</td>
<td>PCSORSetIIts()</td>
<td>-pcSOR_iits &lt;its&gt;</td>
</tr>
<tr>
<td>Set SOR parameter</td>
<td>PCSORSetOmega()</td>
<td>-pcSOR_omega &lt;omega&gt;</td>
</tr>
<tr>
<td>Set additive Schwarz variant</td>
<td>PCASMSetType()</td>
<td>-pc_asm_type [basic,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>restrict,interpolate,none]</td>
</tr>
<tr>
<td>Set subdomain solver options</td>
<td>PCGetSubSLES()</td>
<td>-sub_pc_type &lt;pctype&gt;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-sub_ksp_type</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-ksp_krylov_type &lt;krylov_type&gt;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-sub_ksp_rtol &lt;rtol&gt;</td>
</tr>
</tbody>
</table>

And many more options...

<table>
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<tr>
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<tr>
<th>Functionality</th>
<th>Procedural Interface</th>
<th>Runtime Option</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set Krylov method</td>
<td>KSPSetType()</td>
<td>-ksp_type [cg, gmres,bcgs,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>tfqmr,cgs,...]</td>
</tr>
<tr>
<td>Set monitoring routine</td>
<td>KSPSetMonitor()</td>
<td>-ksp_monitor, -ksp_xmonitor,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-ksp_truemonitor,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-ksp_xtruemonitor</td>
</tr>
<tr>
<td>Set convergence tolerances</td>
<td>KSPSetTolerances()</td>
<td>-ksp_rtol &lt;rt&gt; -ksp_atol &lt;at&gt;</td>
</tr>
<tr>
<td>Set GMRES restart parameter</td>
<td>KSPGMRESSetRestart()</td>
<td>-ksp_max_iits &lt;iits&gt;</td>
</tr>
<tr>
<td>Set orthogonalization routine for GMRES</td>
<td>KSPGMRESSetOrthogonalization()</td>
<td>-ksp_unmodifiedgramschtmd</td>
</tr>
<tr>
<td></td>
<td></td>
<td>-ksp_irorthog</td>
</tr>
</tbody>
</table>

And many more options...

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SLES: Example Programs

Location: petsc/src/sles/examples/tutorials/

- ex1.c, ex1f.F - basic uniprocessor codes
- ex23.c - basic parallel code
- ex11.c - using complex numbers
- ex4.c - using different linear system and preconditioner matrices
- ex9.c - repeatedly solving different linear systems
- ex22.c - 3D Laplacian using multigrid
- ex15.c - setting a user-defined preconditioner

And many more examples ...

### Conclusion

- Summary
- Interfacing with other packages
- Extensibility issues
- References
Summary

• Creating data objects
• Setting algorithmic options for linear, nonlinear and ODE solvers
• Using callbacks to set up the problems for nonlinear and ODE solvers
• Managing data layout and ghost point communication
• Evaluating parallel functions and Jacobians
• Consistent profiling and error handling

Using PETSc with Other Packages

• Linear algebra solvers
  – AMG
  – BlockSolve95
  – ILUTP
  – LUSOL
  – SPAI
  – SuperLU
• Optimization software
  – TAO
  – Veltisto
• Mesh and discretization tools
  – Overture
  – SAMRAI
  – SUMAA3d
• ODE solvers
  – PVODE
• Others
  – Matlab
  – ParMETIS
Using PETSc with Other Packages:
Linear Solvers

• AMG
  - Algebraic multigrid code by J. Ruge, K. Steuben, and R. Hempel (GMD)
  - [http://www.mgnet.org/mgnet-codes-gmd.html](http://www.mgnet.org/mgnet-codes-gmd.html)
  - PETSc interface by D. Lahaye (K.U.Leuven), uses MatSeqAIJ

• BlockSolve95
  - Parallel, sparse ILU(0) for symmetric nonzero structure and ICC(0)
  - M. Jones (Virginia Tech.) and P. Plassmann (Penn State Univ.)
  - [http://www.mcs.anl.gov/BlockSolve95](http://www.mcs.anl.gov/BlockSolve95)
  - PETSc interface uses MatMPIRowbs

• ILUTP
  - Drop tolerance ILU by Y. Saad (Univ. of Minnesota), in SPARSKIT
  - PETSc interface uses MatSeqAIJ

• LUSOL
  - Sparse LU, part of MINOS
  - M. Saunders (Stanford Univ)
  - [http://www.sbsi-sol-optimize.com](http://www.sbsi-sol-optimize.com)
  - PETSc interface by T. Munson (ANL), uses MatSeqAIJ

• SPAI
  - Sparse approximate inverse code by S. Barnhard (NASA Ames) and M. Grote (ETH Zurich)
  - PETSc interface converts from any matrix format to SPAI matrix

• SuperLU
  - Parallel, sparse LU
  - J. Demmel, J. Gilbert, (U.C. Berkeley) and X. Li (NERSC)
  - [http://www-users.nersc.gov/~xiaoye/SuperLU](http://www-users.nersc.gov/~xiaoye/SuperLU)
  - PETSc interface uses MatSeqAIJ
  - Currently only sequential interface supported; parallel interface under development
Using PETSc with Other Packages:
TAO – Optimization Software

- TAO - Toolkit for Advanced Optimization
  - Software for large-scale optimization problems
  - S. Benson, L. McInnes, and J. Moré
  - [http://www.mcs.anl.gov/tao](http://www.mcs.anl.gov/tao)
- Initial TAO design uses PETSc for
  - Low-level system infrastructure - managing portability
  - Parallel linear algebra tools (SLES)
    - Veltisto (library for PDE-constrained optimization by G. Biros, see [http://www.cs.nyu.edu/~biros/veltisto](http://www.cs.nyu.edu/~biros/veltisto)) uses a similar interface approach
- TAO is evolving toward
  - CCA-compliant component-based design (see [http://www.cca-forum.org](http://www.cca-forum.org))
  - Support for ESI interfaces to various linear algebra libraries (see [http://z.ca.sandia.gov/esi](http://z.ca.sandia.gov/esi))

Using PETSc with Other Packages:
PVODE – ODE Integrators

- PVODE
  - Parallel, robust, variable-order stiff and non-stiff ODE integrators
  - A. Hindmarsh et al. (LLNL)
  - [http://www.llnl.gov/CASC/PVODE](http://www.llnl.gov/CASC/PVODE)
  - L. Xu developed PVODE/PETSc interface
- Interface Approach
  - PVODE
    - ODE integrator – evolves field variables in time
    - vector – holds field variables
    - preconditioner placeholder
  - PETSc
    - ODE integrator placeholder
    - vector
    - sparse matrix and preconditioner
- Usage
  - TSCreate(MPI_Comm,TS_NONLINEAR,&ts)
  - TSBindVector(ts,TS_PVODE)
  - …… regular TS functions
  - TSPVODESetType(ts,PVODE_ADAMS)
  - …… other PVODE options
  - TSSetFromOptions(ts) – accepts PVODE options
Using PETSc with Other Packages:

Mesh Management and Discretization

• SUMAA3d
  – Scalable Unstructured Mesh Algorithms and Applications
  – L. Freitag (ANL), M. Jones (VA Tech), P. Plassmann (Penn State)
  – http://www.mcs.anl.gov/sumaa3d
  – L. Freitag and M. Jones developed SUMAA3d/PETSc interface

• SAMRAI
  – Structured adaptive mesh refinement
  – R. Hornung, S. Kohn (LLNL)
  – http://www.llnl.gov/CASC/SAMRAI
  – SAMRAI team developed SAMRAI/PETSc interface

• Overture
  – Structured composite meshes and discretizations
  – D. Brown, W. Henshaw, D. Quinlan (LLNL)
  – http://www.llnl.gov/CASC/Overture
  – K. Buschelman and Overture team developed Overture/PETSc interfaces

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Using PETSc with Other Packages:

Matlab

• Matlab
  – http://www.mathworks.com

• Interface Approach
  – PETSc socket interface to Matlab
    – Sends matrices and vectors to interactive Matlab session
  – PETSc interface to MatlabEngine
    – MatlabEngine – Matlab library that allows C/Fortran programmers to use Matlab functions in programs
    – PetscMatlabEngine – unwraps PETSc vectors and matrices so that MatlabEngine can understand them

• Usage
  – PetscMatlabEngineCreate(MPI_Comm, machinename, PetscMatlabEngine eng)
  – PetscMatlabEnginePut(eng, PetscObject obj)
    – Vector
    – Matrix
  – PetscMatlabEngineEvaluate(eng, "R = QR(A);")
  – PetscMatlabEngineGet(eng, PetscObject obj)
Using PETSc with Other Packages:
ParMETIS – Graph Partitioning

• ParMETIS
  – Parallel graph partitioning
  – G. Karypis (Univ. of Minnesota)
  – http://www.cs.umn.edu/~karypis/metis/parmetis

• Interface Approach
  – Use PETSc MatPartitioning() interface and MPIAIJ or MPIAdj matrix formats

• Usage
  – MatPartitioningCreate(MPI_Comm,MatPartitioning ctx)
  – MatPartitioningSetAdjacency(ctx,matrix)
  – Optional – MatPartitioningSetVertexWeights(ctx,weights)
  – MatPartitioningSetFromOptions(ctx)
  – MatPartitioningApply(ctx,IS *partitioning)

Extensibility Issues

• Most PETSc objects are designed to allow one to “drop in” a new implementation with a new set of data structures (similar to implementing a new class in C++).

• Heavily commented example codes include
  – Krylov methods: petsc/src/sles/ksp/impls/cg
  – preconditioners: petsc/src/sles/pc/impls/jacobi

• Feel free to discuss more details with us in person.
Caveats Revisited

- Developing parallel, non-trivial PDE solvers that deliver high performance is still difficult, and requires months (or even years) of concentrated effort.
- PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver nor a silver bullet.
- Users are invited to interact directly with us regarding correctness and performance issues by writing to petsc-maint@mcs.anl.gov.

References

  - PETSc Users manual
  - Manual pages
  - Many hyperlinked examples
  - FAQ, Troubleshooting info, installation info, etc.
  - Research and publications that make use PETSc
- MPI Information: [http://www.mpi-forum.org](http://www.mpi-forum.org)
- *Using MPI* (2nd Edition), by Gropp, Lusk, and Skjellum
- *Domain Decomposition*, by Smith, Bjorstad, and Gropp