Building a Successful Scalable Parallel Numerical Library: Lessons From the PETSc Library

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What is PETSc?

- PETSc is a numerical library that is organized around mathematical concepts appropriate for the solution of linear and nonlinear systems of equations that arise from discretizations of Partial Differential Equations
- PETSc began as a tool to aid in research into domain decomposition methods for elliptic and hyperbolic (with implicit time stepping) partial differential equations. A new library was needed because
  - Numerical libraries of the time were organized around particular algorithms, rather than mathematical problems, making experimentation with different algorithms difficult
  - Most libraries were not re-entrant, making recursive use impossible
- PETSc addressed these limitations and clearly filled a need; PETSc is now used by both applications scientists and researchers (100's of users including DOE and NSF leadership computing platforms)

The PETSc Team (Past and Present)


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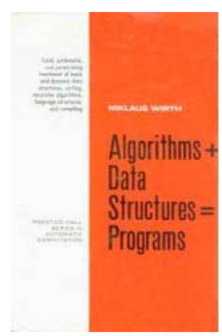
Everyone contributed to the results described in this talk

How Should Numerical Libraries Be Designed?



- It is common to choose an algorithms and a data structure
  - "Algorithms + Data Structures = Programs"
- Rarely unique choices
- Better is to say: I'm solving Ax=b
  - PETSc really looks at F(x,t) = 0, for which Ax=b is a key component
- Lets look at the Ax=b part…

The Constraints - Parallel Computing Issues

- Distributed Memory Model
  - Programmer must participate in handling decomposition of objects across processes
- Shared Memory Model
  - Poor integration with language (race detection, volatile, lack of write/read barriers)
  - Difficult to achieve scalability (hardware costly, complicated)
- Consequences
  - Choose MPI distributed memory model
  - Would do the same today
    - But maybe PGAS language will be appropriate soon
  - Scalability requires careful attention to message latency

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Distributed Objects

- PETSc must provide a mechanism to work with objects that are distributed across a collection of processors
- Common patterns:
  - Err = <THING>Create(parallel-context,<INFO>, <SIZE>, &object)
  - Err = <THING>Destroy(object)
    Err = <THING><Operation>(object, <other-parms>)
- For example,
  - VecCreate(MPI_COMM_WORLD, PETSC_DECIDE, n, &x)
  - MatMult(A, x, y)
- Operations use the same name when possible:
  - <THING>SetFromOptions(object)
    - Use command line, environment variables, or defaults file to set basic properties

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Vectors in PETSc

- Mathematical Objects
  - *Not* a contiguous section of memory
- Distributed across a set of processes
  - May be a subset of all processes in the parallel job
  - First decision:
    - How general a distribution is allowed for the representation of data?
    - For example, should ghost cells be allowed? Non-contiguous sections?
  - PETSc uses a very simple decomposition
    - A single, contiguous segment, ordered with the rank of the processes
    - Chosen for performance
  - Lesson 1: Permit the best performance

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Does PETSc Need More General Vectors?

- So, how do you handle more general decompositions? PETSc provides several alternatives, depending on the type of generality
  - Non-contiguous in process: copy
    - Not as bad as it seems, as the copy may provide better cache locality and not be that costly
  - Non-contiguous across processes: permutations
    - Often better to apply permutations, then use
  - Plus, PETSc allows the use of arbitrary representations for vectors
    - But then the user is responsible for implementing all operations between vectors, and operations on vectors by other objects, such as matrix-vector product
  - Lesson 2: Provide an escape for customization

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Accessing Elements of a Vector

- The element-wise approach seems simple:
  - V[k] = 3
- But what is involved with this in a parallel computer?
  - One possibility is:
    - Retrieve cache line containing v[k] from the current owner of that cache line if any, assert ownership (flush from owner's cache)
    - Update the bytes corresponding to V[k].
    - Write out the data to memory
    - When the original owner needs to access (even to read), figure out if the ownership of the cache line should move
    - !!!!
  - There are other options, but they all must handle where data is cached and how it is updated.
- Is this a good operation to support?
  - Rarely a natural mathematical operation
  - E.g., usually define entire vector, as in v = f(x,y)
  - Setting a single element in a vector is both costly and rarely necessary

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Improving Performance of Vector Element Update

- Lesson 3: Define/Update objects as a single operation
  - Defer the "synchronization"; v[k] tells the language that after the assignment, v[k] is visible anywhere v is defined. This may force the system to wait until the data is available or to implement complex caching strategies
  - The alternative is relaxed consistency models, which may lead the programmer to refer to data before it is available (because of a mismatch between the computer language and these memory consistency models)
- Instead, define an operation that allows the user to define when the object must be ready for use. This is a simple generalization of the notion of matrix assembly

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Assembly

- PETSc uses the notion of object assembly
  - First, describe update
  - Initiate assembly
    - Allow other work (Communication/Computation Overlap)
    - At least, that was the theory:
      - Communication systems require extra hardware support to effectively overlap communication and computation
      - There may not be natural work to insert in this slot
  - Wait for the assembly to complete
    - Note: still introduces more synchronization than strictly required (there are possibilities here for improvement)
    - This model selected for its simplicity
- This applies to all objects that must be assembled
- Not a new idea
  - Same idea used to vectorize sparse matrix assembly
    - Same problem - single element updates do not fit vector model

Setting Elements of a Vector

- While changing the vector so that a single element is updated is inefficient, it is simple
- PETSc provides a way to "set/add to an element that will be visible after the assembly completes":
  - VecSetValue( )
- Since many multicomponent PDEs naturally compute/update all the values at a grid point
  - VecSetValues()
- Key features:
  - Values set are in the mathematical vector object
    - User need not know/understand decomposition of vector representation across processes
  - Values are not available until after Assembly step completes
  - PETSc efficiently manages the implementation of assembly
    - Caches data, aggregates values destined to the same process
    - Transparent to the user
- Lesson 4: Provide ease-of-use features, even if they are not high-performance. Note that this is not inconsistent with Lesson 1 (permit high performance).

Matrices

- What are PETSc matrices?
  - Fundamental objects for storing linear operators (e.g., Jacobians)
- Create matrices via
  - MatCreate(...,Mat *)
    - MPI_Comm - processes 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: MPISBAIJ, SAEQSBAIJ
      - block diagonal: MPIBDIAG, SEQBDIAG
      - dense: MPIDENSE, SEQDENSE
      - matrix-free
      - etc.
    - MatSetFromOptions(Mat) lets you set the MatType at runtime.

Matrices and Polymorphism

- Single user interface independent of the underlying sparse data structure, 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.

Matrices in PETSc

- A matrix is defined by its properties and the operations that you can perform with it.
  - Not by its data structures
  - (Some operations require efficient access to matrix elements; that only means that some operations, such as incomplete factor, may not be available if the matrix uses a matrix-free representation)
- The ability to associate different code for the same abstract operation, depending on the circumstances (such as the data structure) is called polymorphism. It is a critical part of the PETSc implementation approach
  - Typically implemented with a function pointer

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What Advantage Does This Approach Give You?

- Example: A Poisson Solver in PETSc
  - The following 7 slides show a complete 2-d Poisson solver in PETSc. Features of this solver:
    - Fully parallel
    - 2-d decomposition of the 2-d mesh
    - Linear system described as a sparse matrix; user can select many different sparse data structures
    - Linear system solved with any user-selected Krylov iterative method and preconditioner provided by PETSc, including GMRES with ILU, BiCGstab with Additive Schwarz, etc.
    - Complete performance analysis built-in
  - Only 7 slides of code!

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Solve a Poisson Problem with Preconditioned GMRES

```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
#include <math.h>
#include "petscsles.h"
#include "petscda.h"
extern Mat FormLaplacianDA2d( DA, int );
extern Vec FormVecFromFunctionDA2d( DA, int, double (*)(double,double) );
/* This function is used to define the right-hand side of the
   Poisson equation to be solved */
double func( double x, double y ) {
    return sin(x*M_PI)*sin(y*M_PI); }

int main( int argc, char *argv[] )
{
    SLES      sles;
    Mat       A;
    Vec       b, x;
    DA        grid;
    int       its, n, px, py, worldSize;

    PetscInitialize( &argc, &argv, 0, 0 );
```

PETSC "objects" hide details of distributed data structures and function parameters

```
    /* Get the mesh size.  Use 10 by default */
    n = 10;
    PetscOptionsGetInt( PETSC_NULL, "-n", &n, 0 );
    /* Get the process decomposition.  Default it the same as without
       DAs */
    px = 1;
    PetscOptionsGetInt( PETSC_NULL, "-px", &px, 0 );
    MPI_Comm_size( PETSC_COMM_WORLD, &worldSize );
    py = worldSize / px;

    /* Create a distributed array */
    DACreate2d( PETSC_COMM_WORLD, DA_NONPERIODIC, DA_STENCIL_STAR,
                n, n, px, py, 1, 1, 0, 0, &grid );

    /* Form the matrix and the vector corresponding to the DA */
    A = FormLaplacianDA2d( grid, n );
    b = FormVecFromFunctionDA2d( grid, n, func );
    VecDuplicate( b, &x );
```

PETSc provides routines to access parameters and defaults

PETSc provides routines to create, allocate, and manage distributed data structures

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

PetscPrintf( PETSC_COMM_WORLD, "Solution is:\n" );
VecView( x, PETSC_VIEWER_STDOUT_WORLD );
PetscPrintf( PETSC_COMM_WORLD, "Required %d iterations\n", its );

MatDestroy( A ); VecDestroy( b ); VecDestroy( x );
SLESDestroy( sles ); DADestroy( grid );
PetscFinalize( );
return 0;
}
```

PETSc provides routines that solve systems of sparse linear (and nonlinear) equations

PETSc provides coordinated I/O (behavior is as-if a single process), including the output of the distributed "vec" object

```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
#include "petsc.h"
#include "petscvec.h"
#include "petscda.h"

/* Form a vector based on a function for a 2-d regular mesh on the
   unit square */
Vec FormVecFromFunctionDA2d( DA grid, int n,
                       double (*f)( double, double ) )
{
    Vec    V;
    int    is, ie, js, je, in, jn, i, j;
    double h;
    double **vval;

    h = 1.0 / (n + 1);
    DACreateGlobalVector( grid, &V );

    DAVecGetArray( grid, V, (void **)&vval );
```

```
/* Get global coordinates of this patch in the DA grid */
DAGetCorners( grid, &is, &js, 0, &in, &jn, 0 );
ie = is + in - 1;
je = js + jn - 1;

for (i=is ; i<=ie ; i++) {
            for (j=js ; j<=je ; j++){
              vval[j][i] = (*f)( (i + 1) * h, (j + 1) * h );
            }
  }
  DAVecRestoreArray( grid, V, (void **)&vval );

  return V;
}
```

Almost the uniprocess code

Creating a **Sparse** Matrix, Distributed Across All Processes

```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
#include "petscsles.h"
#include "petscda.h"

/* Form the matrix for the 5-point finite difference 2d Laplacian
   on the unit square. n is the number of interior points along a
   side */
Mat FormLaplacianDA2d( DA grid, int n )
{
    Mat    A;
    int    r, i, j, is, ie, js, je, in, jn, nelm;
    MatStencil cols[5], row;
    double     h, oneByh2, vals[5];

    h = 1.0 / (n + 1); oneByh2 = 1.0 / (h*h);

    DAGetMatrix( grid, MATMPIAIJ, &A );
    /* Get global coordinates of this patch in the DA grid */
    DAGetCorners( grid, &is, &js, 0, &in, &jn, 0 );
    ie = is + in - 1;
    je = js + jn - 1;
```

Creates a parallel distributed matrix using compressed sparse row format

```
for (i=is; i<=ie; i++) {
        for (j=js; j<=je; j++){
          row.j = j; row.i = i; nelm = 0;
          if (j - 1 > 0) {
                vals[nelm]   = oneByh2;
                cols[nelm].j = j - 1; cols[nelm++].i = i;}
          if (i - 1 > 0) {
                vals[nelm]   = oneByh2;
                cols[nelm].j = j;     cols[nelm++].i = i - 1;}
          vals[nelm]   = - 4 * oneByh2;
          cols[nelm].j = j;       cols[nelm++].i = i;
          if (i + 1 < n - 1) {
                vals[nelm]   = oneByh2;
                cols[nelm].j = j;     cols[nelm++].i = i + 1;}
          if (j + 1 < n - 1) {
                vals[nelm]   = oneByh2;
                cols[nelm].j = j + 1; cols[nelm++].i = i;}
          MatSetValuesStencil( A, 1, &row, nelm, cols, vals,
               INSERT_VALUES );
        }
  }

  MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
  MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);

  return A;
}
```

Just the usual code for setting the elements of the sparse matrix (the complexity comes, as it often does, from the boundary conditions)

Computer Science Lessons

- Organize around user-centric concepts
  - PETSc used the mathematics
  - Provide all that is necessary to manage the objects, not just the "key" functions
- Exploit Computer Science techniques to provide that interface
  - Data Encapsulation and Data Hiding
  - Polymorphism
  - Inheritance
- Pay attention to performance

Numerical Analysis Lessons

- Algorithms!
  - ♦ Get the right ones
  - ♦ Get the scalable parallel ones
  - ♦ Note that there is (rarely) a unique best choice
    - Implies that the software must support many algorithms
    - This is why PETSc organized by problems-to-solve rather than algorithms
      - – This may be the most important lesson: Organize by mathematical problem

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Final Comments

- The success of PETSc is due to:
  - ♦ Performance and Scalability
    - Performance is only weakly correlated with FLOPS
  - ♦ Consistent interface based on the mathematical problems
  - ♦ Completeness
    - Can overcome "ease of use"
  - ♦ Attention to portability and configuration issues
    - Particularly for libraries coming from research groups, this is often the critical factor
    - Portability requires care but isn't hard.
- A key advantage to the PETSc approach
  - ♦ Algorithm Independence
    - Until we know the best way, don't make the choice
    - Users can try new algorithms without giving up the ones with which they are comfortable

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