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

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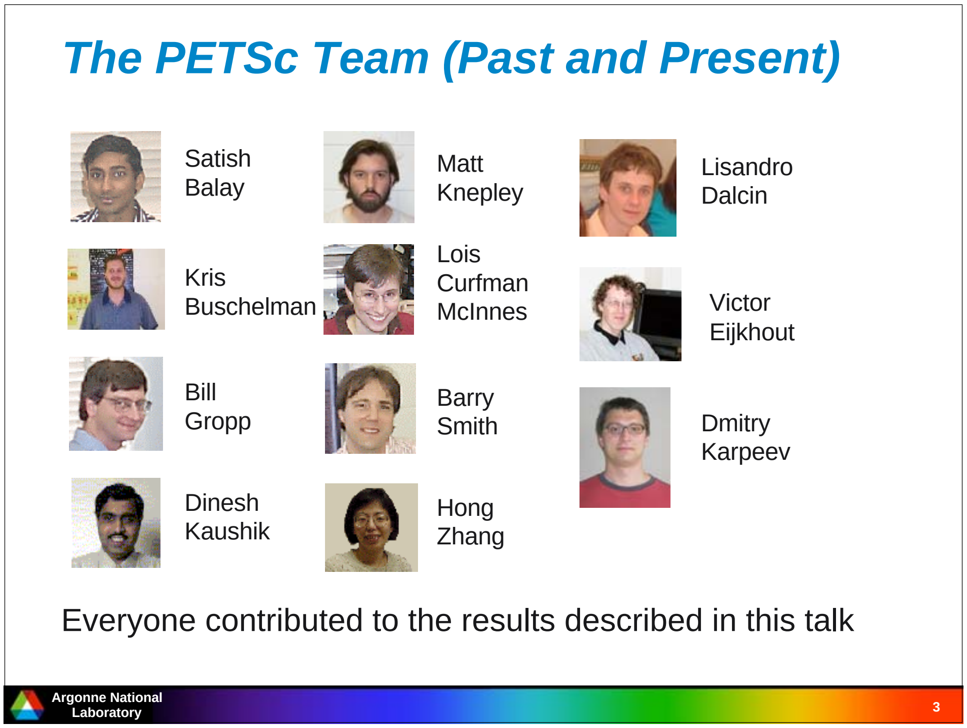
What is PETSc?

- 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



The PETSc Team (Past and Present)

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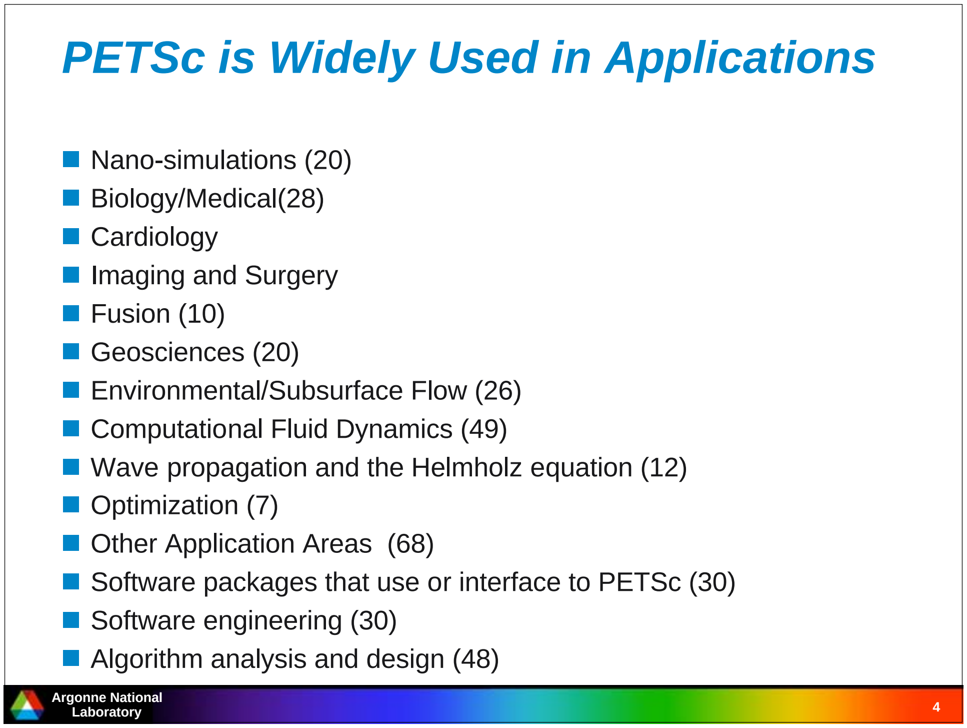
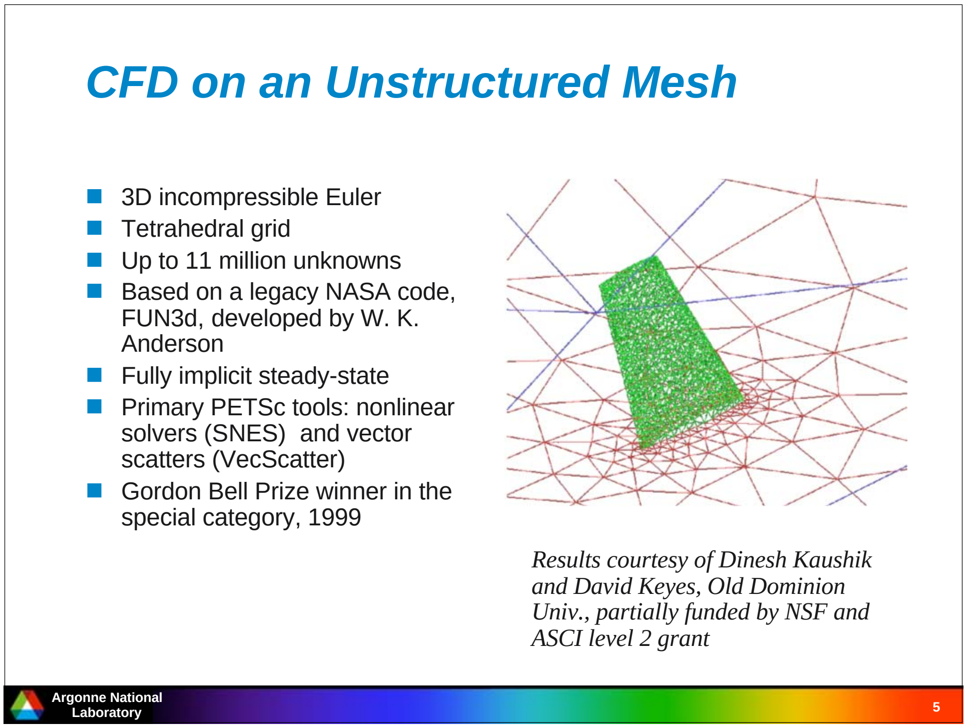
Everyone contributed to the results described in this talk



PETSc is Widely Used in Applications

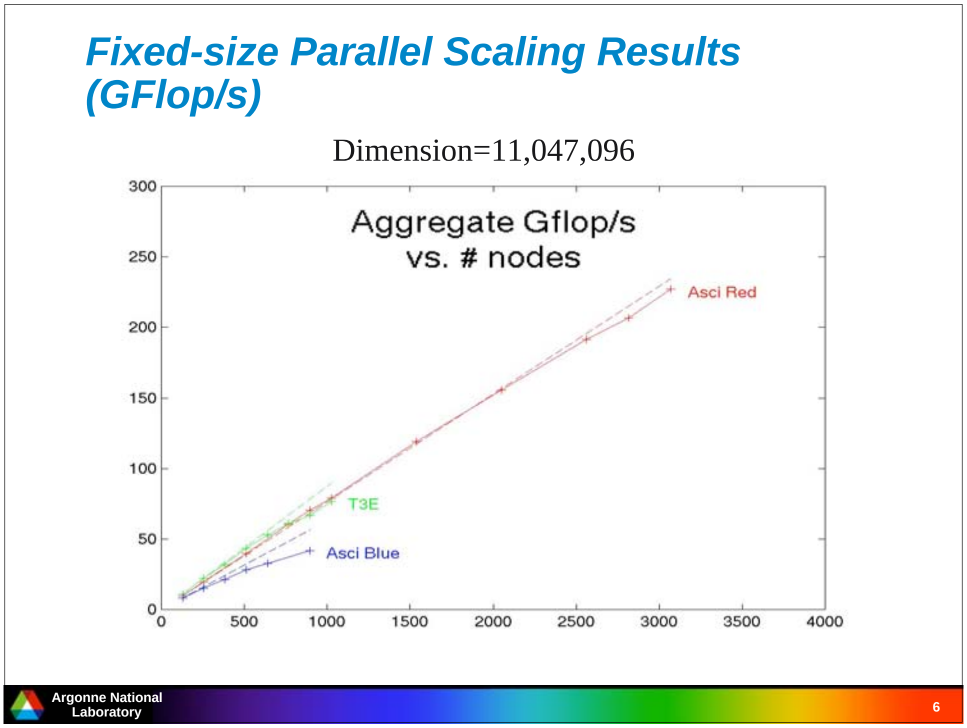
- Nano-simulations (20)
- Biology/Medical(28)
- Cardiology
- Imaging and Surgery
- Fusion (10)
- Geosciences (20)
- Environmental/Subsurface Flow (26)
- Computational Fluid Dynamics (49)
- Wave propagation and the Helmholz equation (12)
- Optimization (7)
- Other Application Areas (68)
- Software packages that use or interface to PETSc (30)
- Software engineering (30)
- Algorithm analysis and design (48)



CFD on an Unstructured Mesh

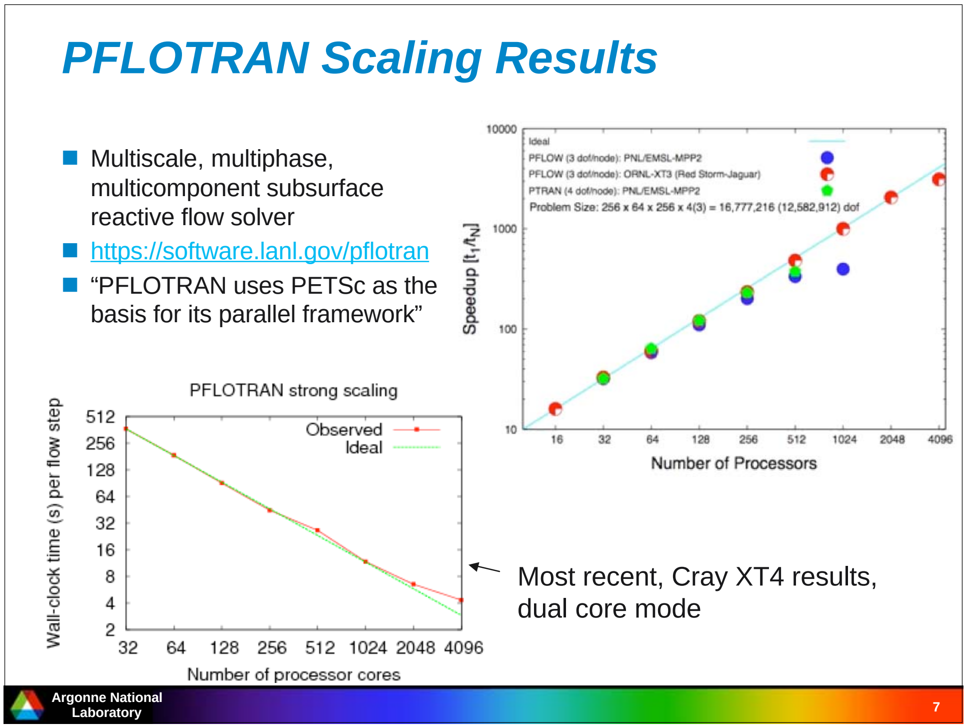
- 3D incompressible Euler
- Tetrahedral grid
- Up to 11 million unknowns
- Based on a legacy NASA code, FUN3d, developed by W. K. Anderson
- Fully implicit steady-state
- Primary PETSc tools: nonlinear solvers (SNES) and vector scatters (VecScatter)
- Gordon Bell Prize winner in the special category, 1999

Results courtesy of Dinesh Kaushik and David Keyes, Old Dominion Univ., partially funded by NSF and ASCI level 2 grant



Fixed-size Parallel Scaling Results (GFlop/s)

Dimension=11,047,096



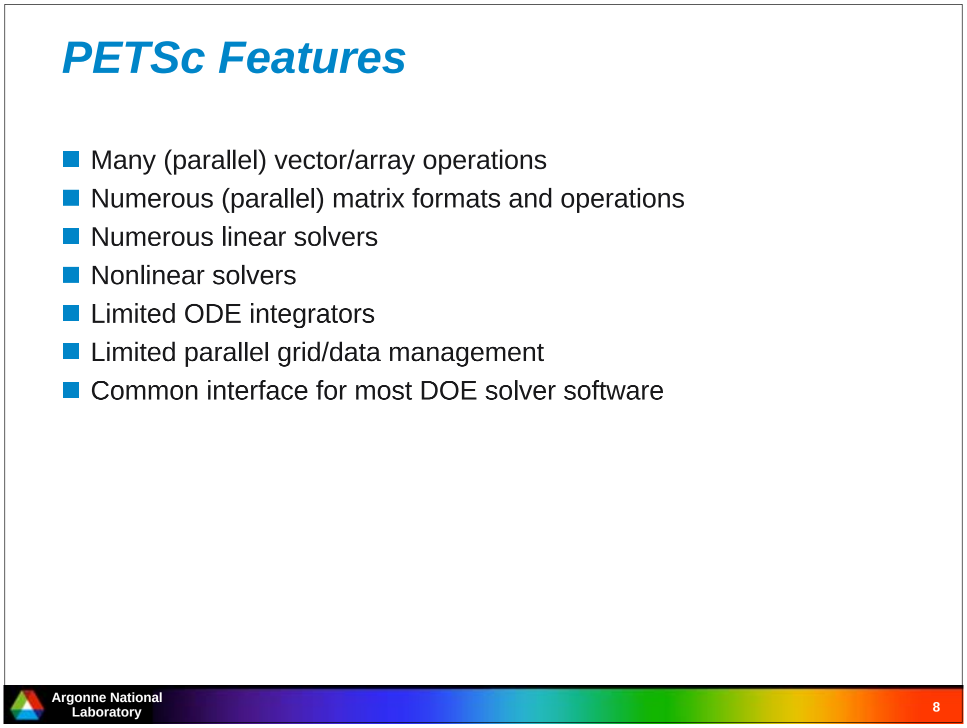
PFLOTRAN Scaling Results

- Multiscale, multiphase, multicomponent subsurface reactive flow solver
- https://software.lanl.gov/pflotran
- “PFLOTRAN uses PETSc as the basis for its parallel framework”

10000
1000
100
10
Speedup [t_1/t_N]
Ideal
PFLOW (3 dof/node): PNL/EMSL-MPP2
PFLOW (3 dof/node): ORNL-XT3 (Red Storm-Jaguar)
PTRAN (4 dof/node): PNL/EMSL-MPP2
Problem Size: 256 x 64 x 256 x 4(3) = 16,777,216 (12,582,912) dof
16
32
64
128
256
512
1024
2048
4096
Number of Processors

PFLOTRAN strong scaling
Wall-clock time (s) per flow step
512
256
128
64
32
16
8
4
2
Observed
Ideal
32
64
128
256
512
1024
2048
4096
Number of processor cores

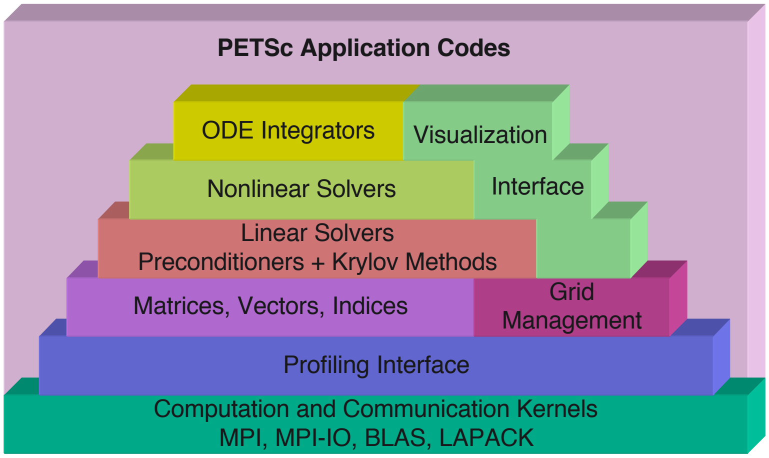
Most recent, Cray XT4 results, dual core mode



PETSc Features

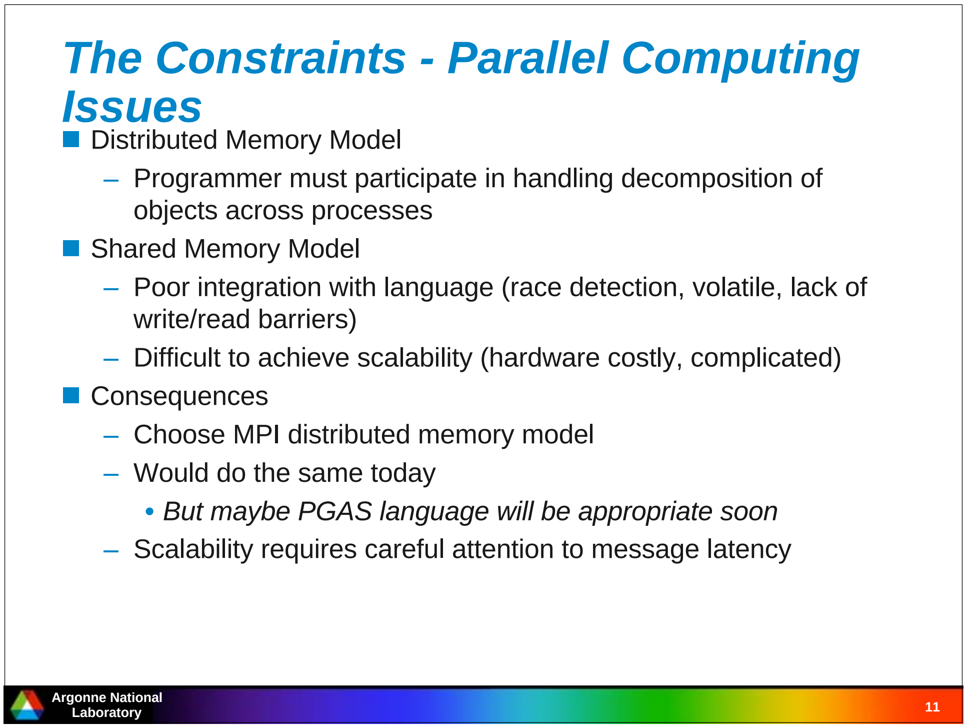
- Many (parallel) vector/array operations
- Numerous (parallel) matrix formats and operations
- Numerous linear solvers
- Nonlinear solvers
- Limited ODE integrators
- Limited parallel grid/data management
- Common interface for most DOE solver software

Structure of PETSc



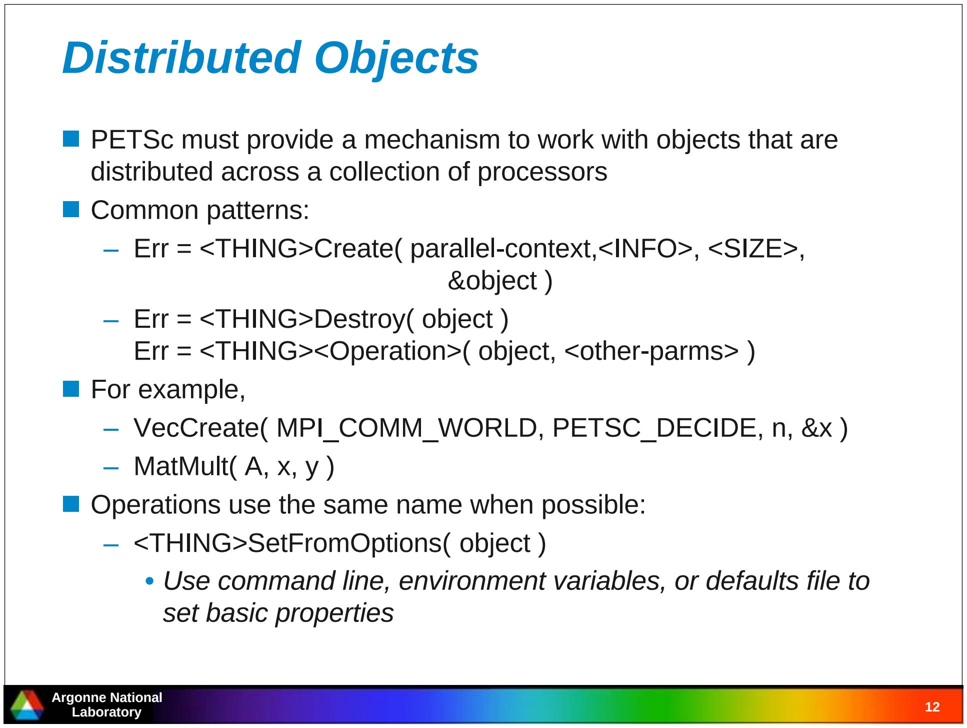
A Journey Through the PETSc Design

- Starting from the constraints on achieving effective parallel and single node performance, I will cover the basic design choices and rationales.
- Then I will show a complete parallel application, complete with performance instrumentation, a wide range of iterative and direct methods, and preconditioners



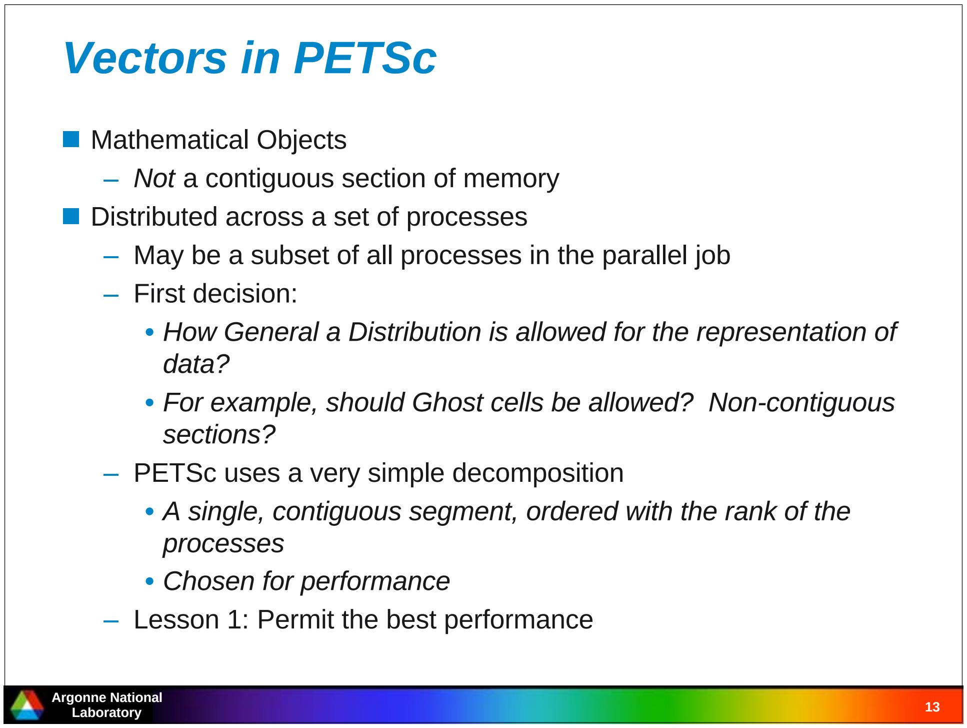
The Constraints - Parallel Computing Issues

- 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



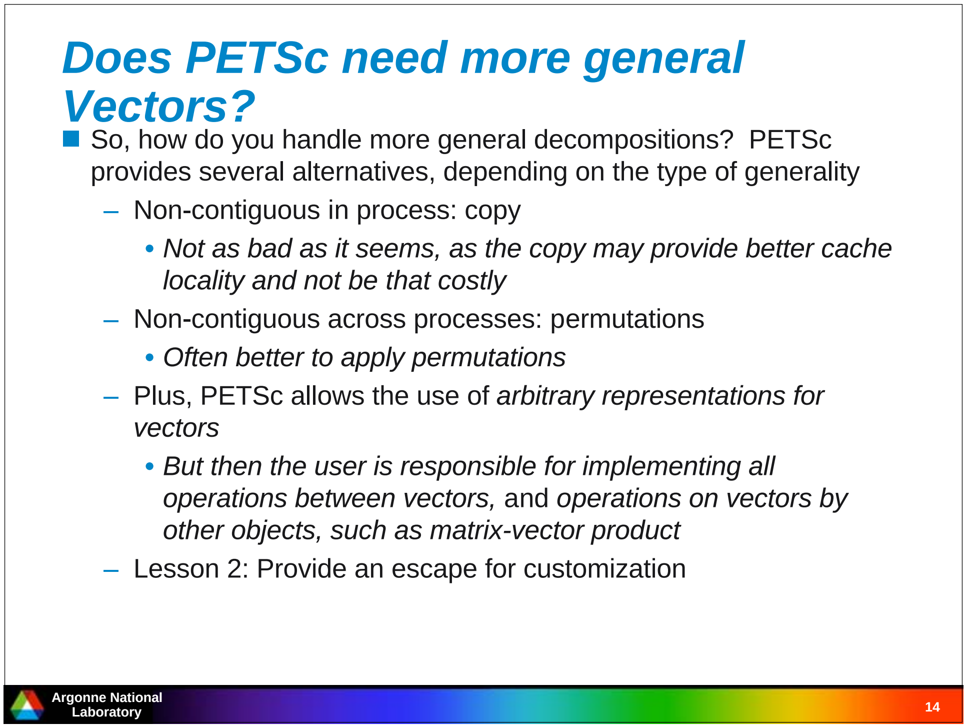
Distributed Objects

- 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*



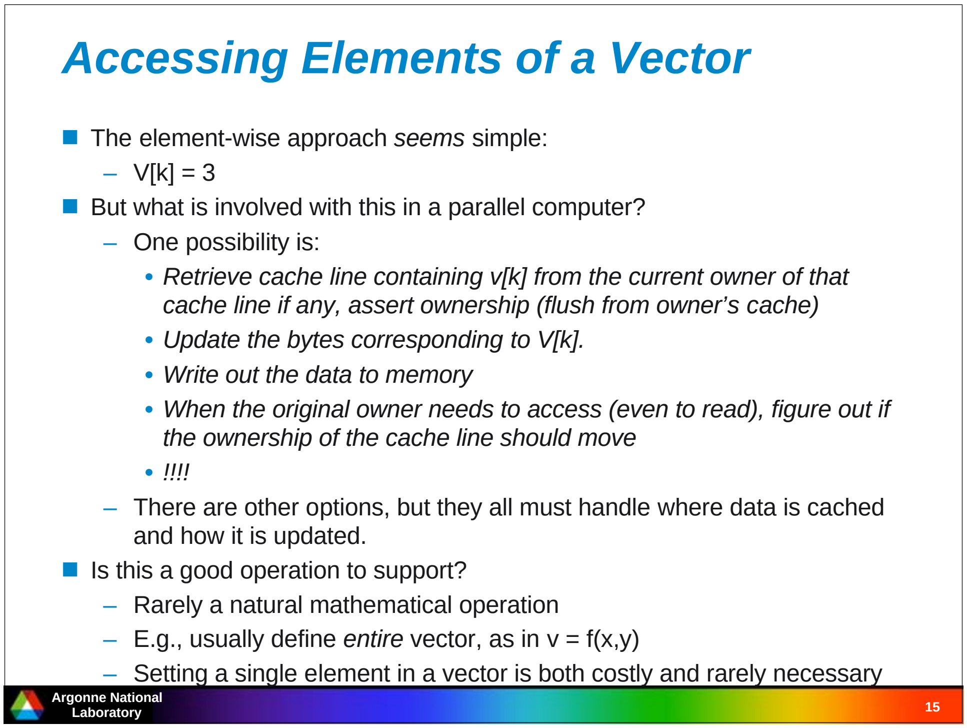
Vectors in PETSc

- 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



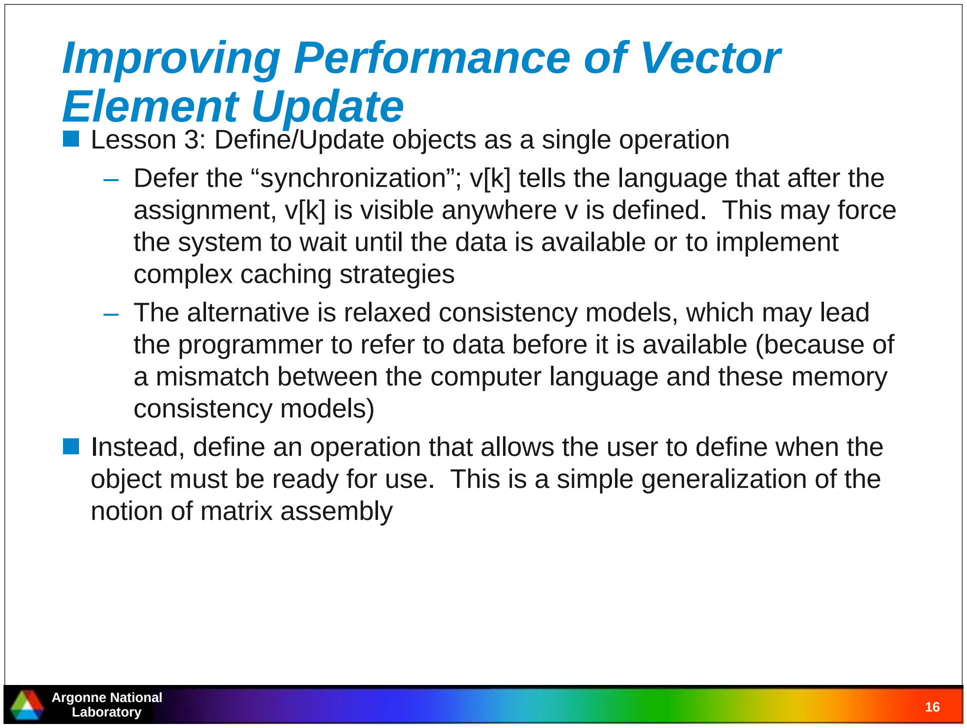
Does PETSc need more general Vectors?

- 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*
  - 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



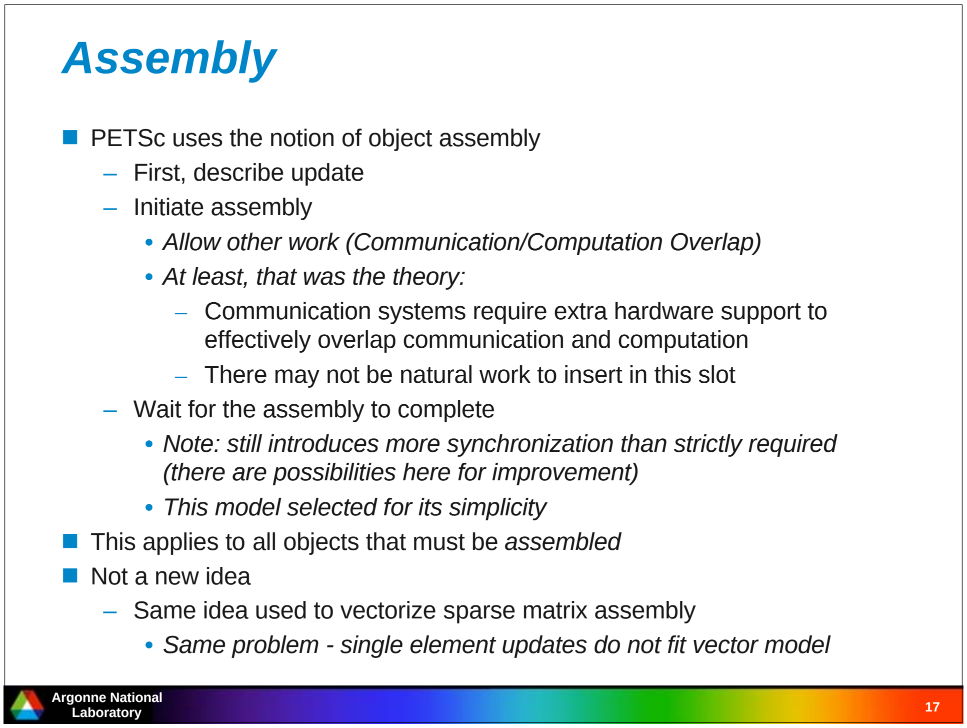
Accessing Elements of a Vector

- 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



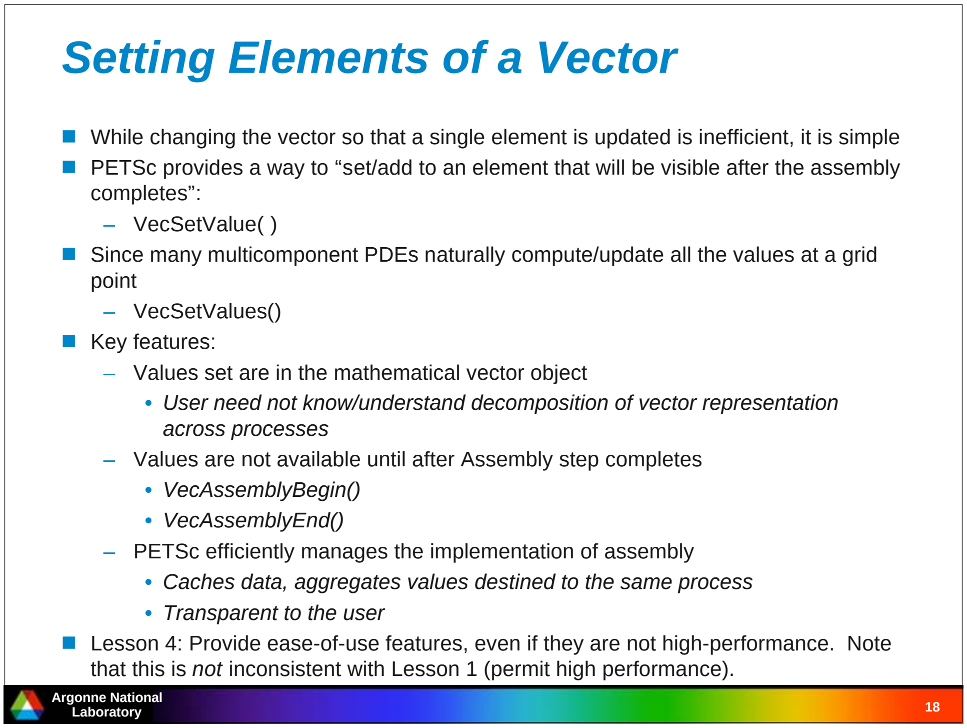
Improving Performance of Vector Element Update

- 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



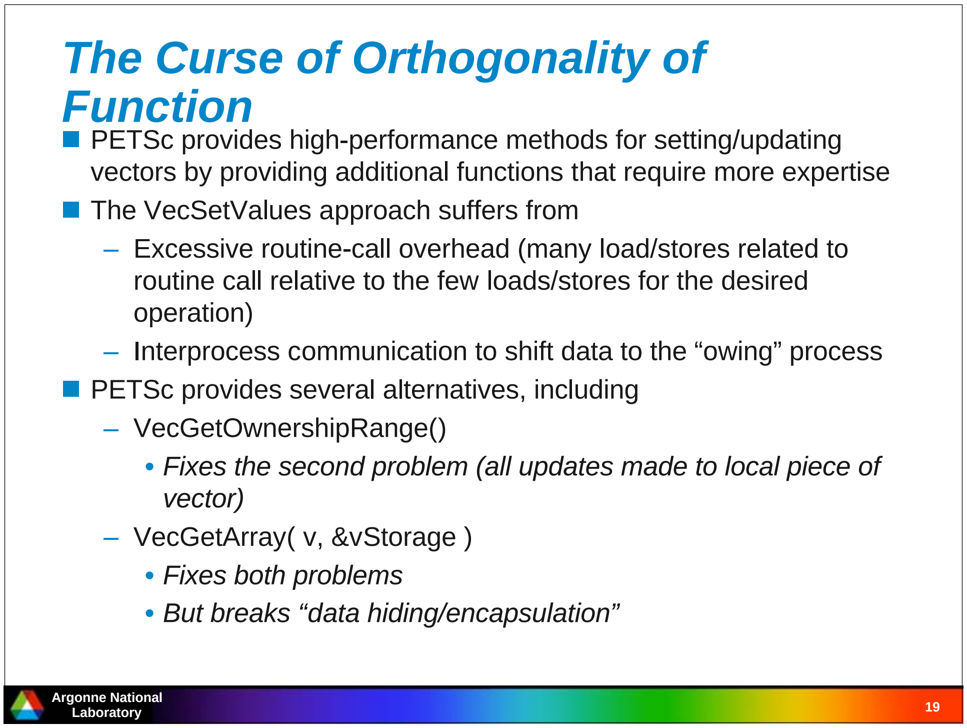
Assembly

- 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
    - *VecAssemblyBegin()*
    - *VecAssemblyEnd()*
  - 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).



The Curse of Orthogonality of Function

- PETSc provides high-performance methods for setting/updating vectors by providing additional functions that require more expertise
- The VecSetValues approach suffers from
  - Excessive routine-call overhead (many load/stores related to routine call relative to the few loads/stores for the desired operation)
  - Interprocess communication to shift data to the “owing” process
- PETSc provides several alternatives, including
  - VecGetOwnershipRange()
    - *Fixes the second problem (all updates made to local piece of vector)*
  - VecGetArray(v, &vStorage)
    - *Fixes both problems*
    - *But breaks “data hiding/encapsulation”*

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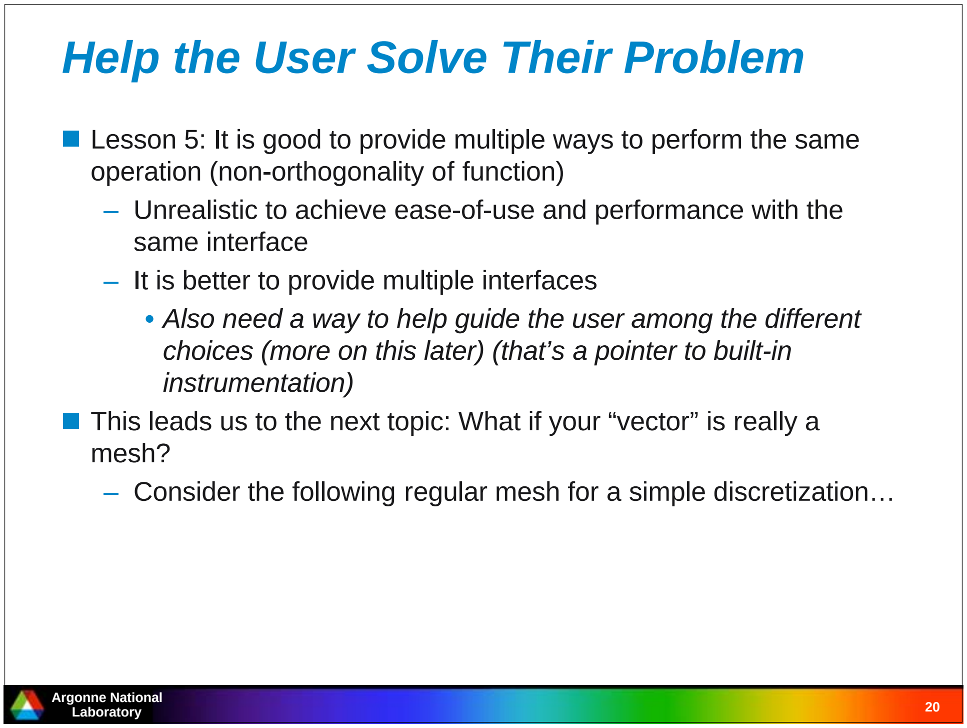

Help the User Solve Their Problem

- Lesson 5: It is good to provide multiple ways to perform the same operation (non-orthogonality of function)
  - Unrealistic to achieve ease-of-use and performance with the same interface
  - It is better to provide multiple interfaces
    - *Also need a way to help guide the user among the different choices (more on this later) (that’s a pointer to built-in instrumentation)*
- This leads us to the next topic: What if your “vector” is really a mesh?
  - Consider the following regular mesh for a simple discretization…

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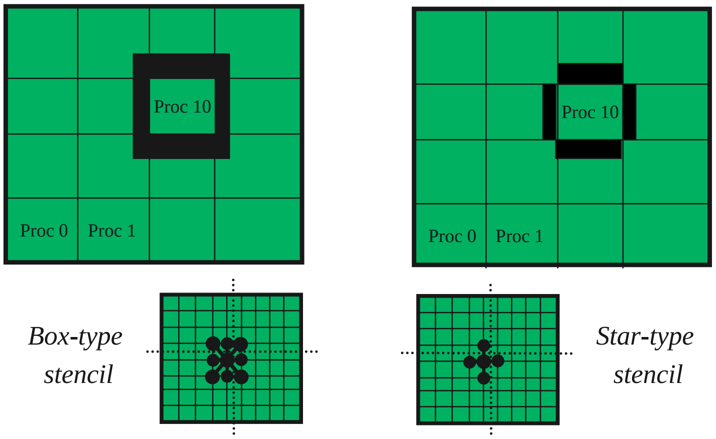
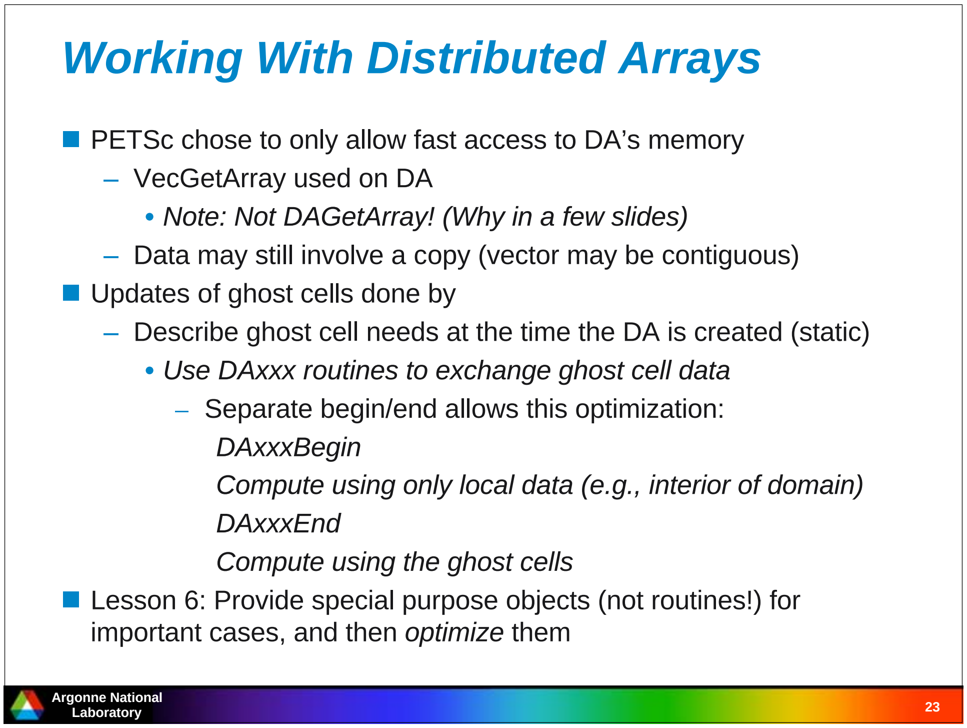
Distributed Arrays With Ghost Cells

Data layout and ghost values



Distributed Arrays as Extensions of Vectors

- PETSc defines a “Distributed Array” which is a
  - Multi-dimensional array
  - Optimized for stencil operations by providing “ghost cells”
- Same Issues as for vectors:
  - Element-wise operations are easy to describe
  - But an application (almost) never applies a stencil to a single point; always to entire (distributed) array
    - *May apply different stencils at different points, but that’s an aggregate operation if done properly*



Working With Distributed Arrays

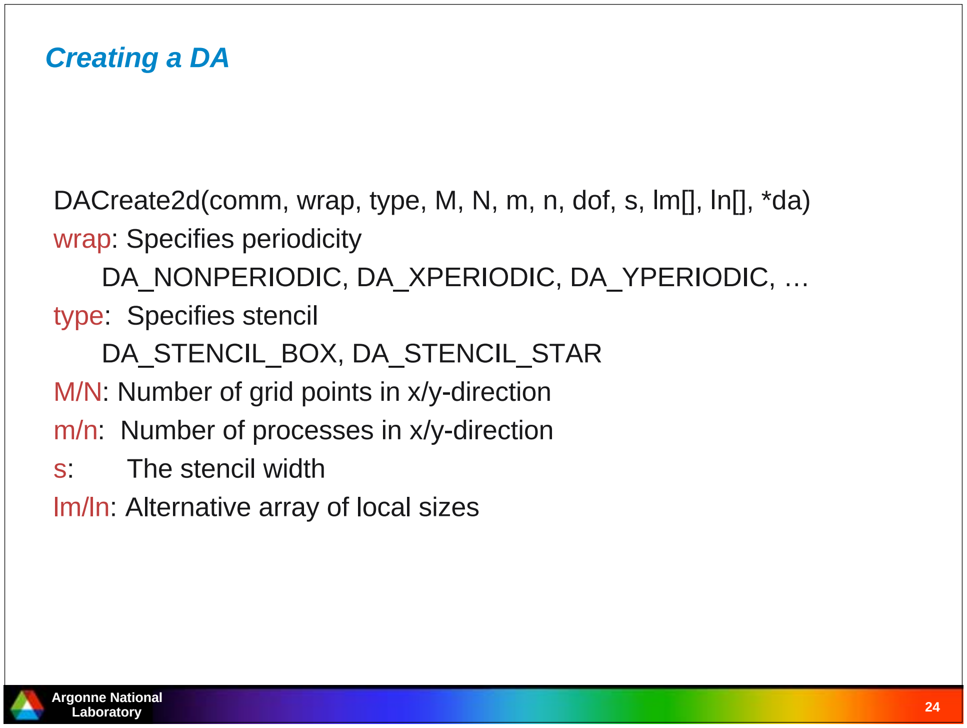
- PETSc chose to only allow fast access to DA's memory
  - VecGetArray used on DA
    - *Note: Not DAGetArray! (Why in a few slides)*
  - Data may still involve a copy (vector may be contiguous)
- Updates of ghost cells done by
  - Describe ghost cell needs at the time the DA is created (static)
    - *Use DAxxx routines to exchange ghost cell data*
      - Separate begin/end allows this optimization:

        DAxxxBegin

        Compute using only local data (e.g., interior of domain)

        DAxxxEnd

        Compute using the ghost cells
- Lesson 6: Provide special purpose objects (not routines!) for important cases, and then *optimize* them



Creating a DA

DACreate2d(comm, wrap, type, M, N, m, n, dof, s, lm[], ln[], *da)

wrap: Specifies periodicity

DA_NONPERIODIC, DA_XPERIODIC, DA_YPERIODIC, …

type: Specifies stencil

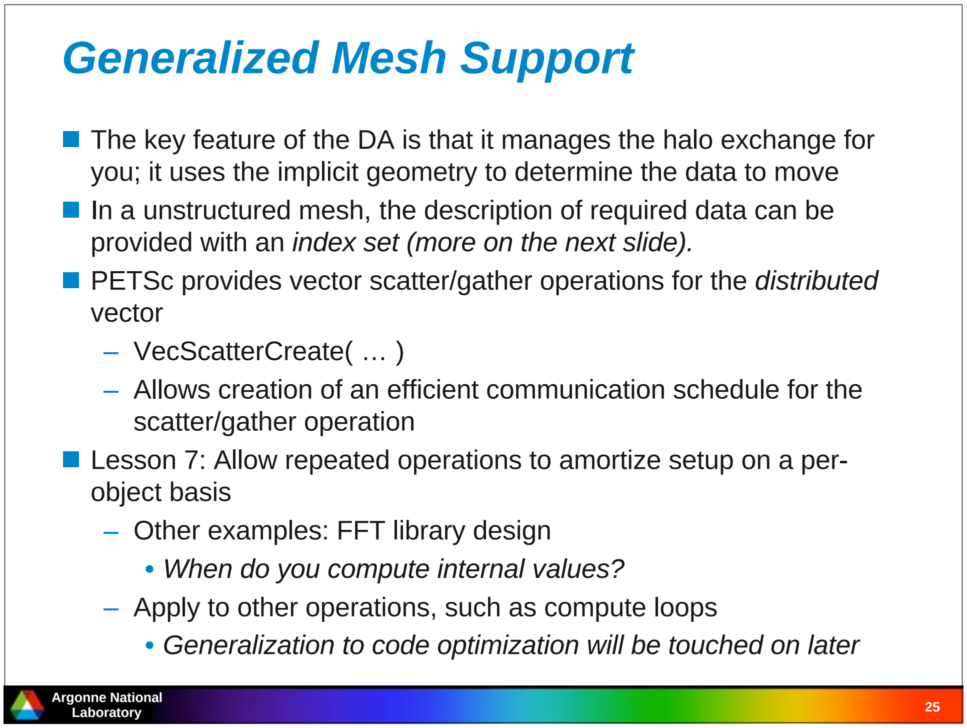
DA_STENCIL_BOX, DA_STENCIL_STAR

M/N: Number of grid points in x/y-direction

m/n: Number of processes in x/y-direction

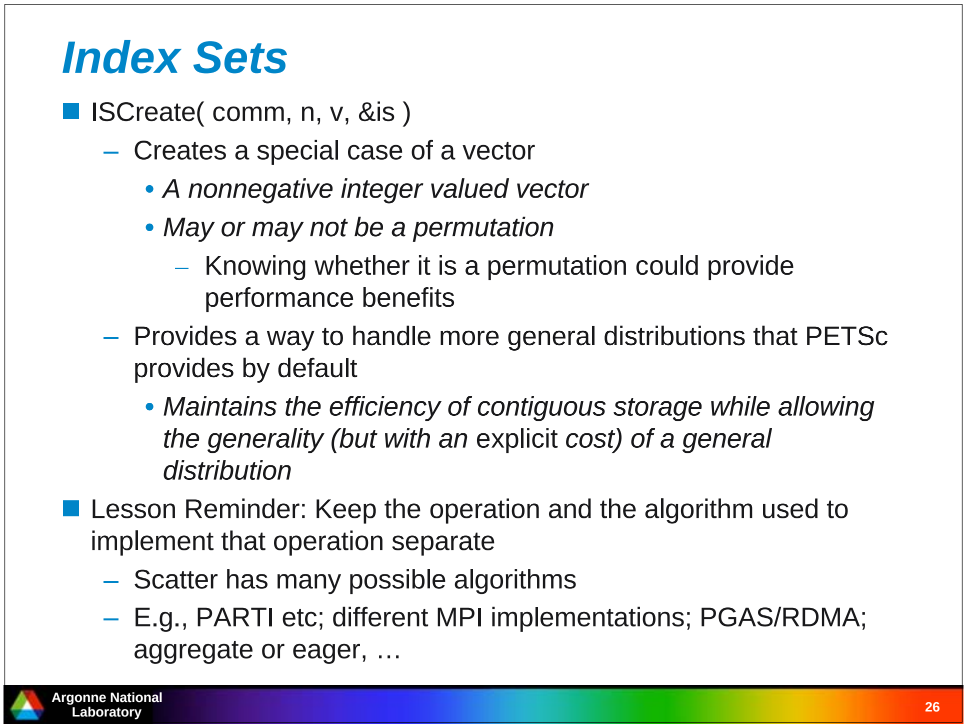
s: The stencil width

lm/ln: Alternative array of local sizes



Generalized Mesh Support

- The key feature of the DA is that it manages the halo exchange for you; it uses the implicit geometry to determine the data to move
- In a unstructured mesh, the description of required data can be provided with an *index set (more on the next slide).*
- PETSc provides vector scatter/gather operations for the *distributed* vector
  - VecScatterCreate(…)
  - Allows creation of an efficient communication schedule for the scatter/gather operation
- Lesson 7: Allow repeated operations to amortize setup on a per-object basis
  - Other examples: FFT library design
    - *When do you compute internal values?*
  - Apply to other operations, such as compute loops
    - *Generalization to code optimization will be touched on later*



Index Sets

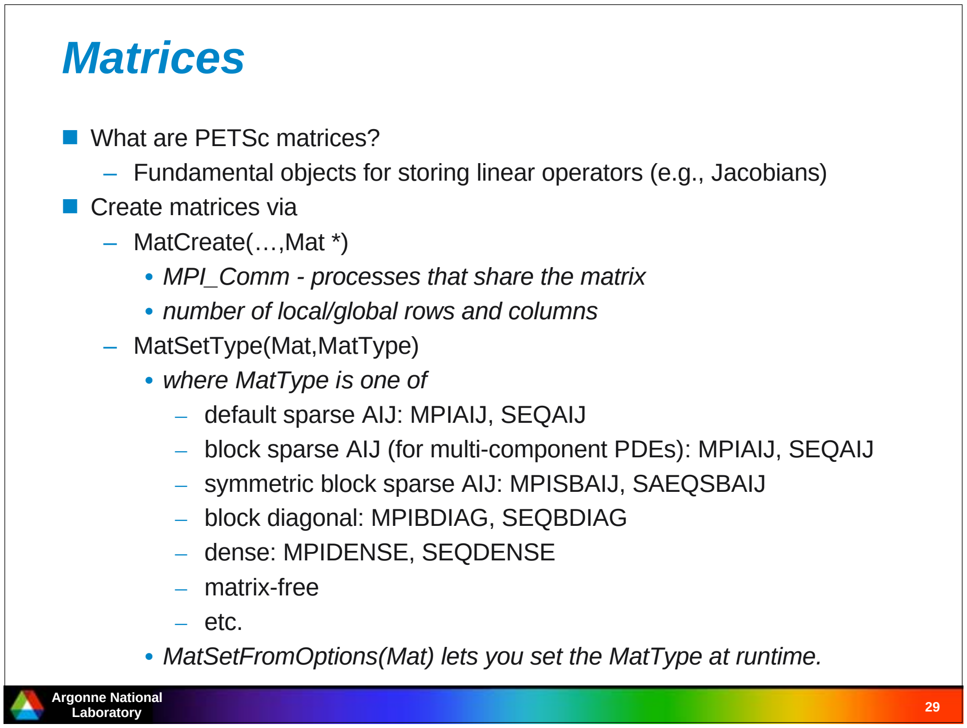
- ISCreate(comm, n, v, &is)
  - Creates a special case of a vector
    - *A nonnegative integer valued vector*
    - *May or may not be a permutation*
      - Knowing whether it is a permutation could provide performance benefits
  - Provides a way to handle more general distributions that PETSc provides by default
    - *Maintains the efficiency of contiguous storage while allowing the generality (but with an* explicit *cost) of a general distribution*
- Lesson Reminder: Keep the operation and the algorithm used to implement that operation separate
  - Scatter has many possible algorithms
  - E.g., PARTI etc; different MPI implementations; PGAS/RDMA; aggregate or eager, …

Object Oriented Design

- Same ideas continue into the Matrix, Linear Solver, Nonlinear Solver, …objects and operations
- This is an example of Object-Oriented Design (O-O)
  - Define the objects (e.g., Matrix) and the operations that act on them (methods)
  - Think of the objects as a class and consider the natural and necessary operations upon them
  - Internal information, such as the data structures used to represent the objects or to efficiently operate upon them, are not exposed to the user of the object (usually)
- O-O provides a implementation strategy for the ideas here
- O-O focuses on the objects, their relationships, and the operations on and between them. The particular code or function *may not be known until run time* (more later)
- O-O can be used in any computer language, though some are easier than others (PETSc is written almost entirely in C)

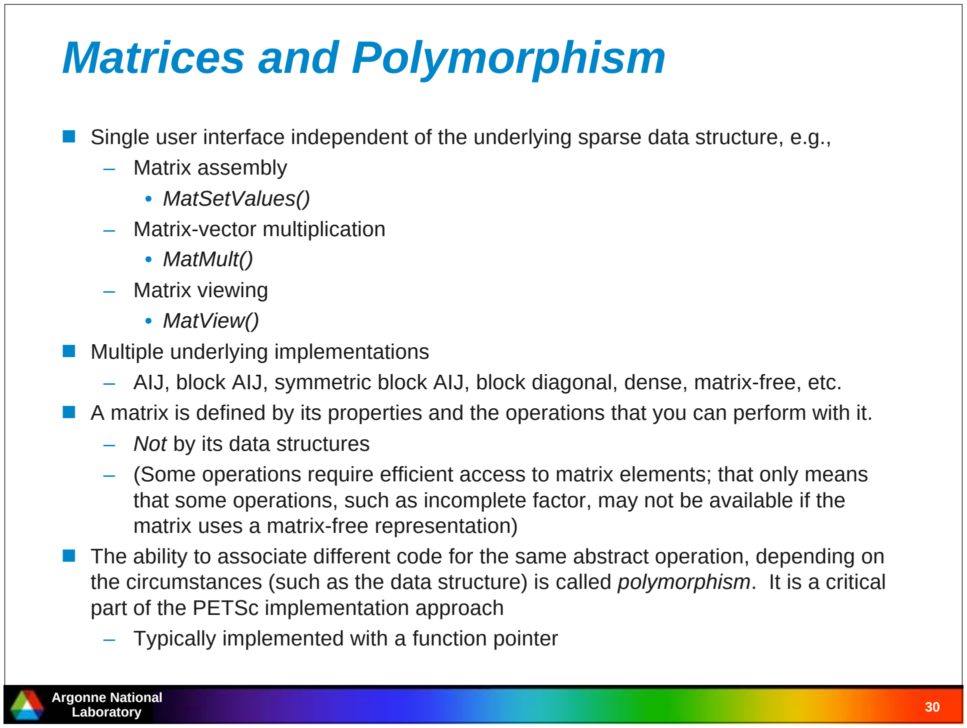
Inheritance

- It is typical that one object is an extension of another
- For example, a discretization mesh is a vector with additional properties, such as the geometric location of each element
- Some operations require this geometric knowledge, e.g., display, geometric-based preconditioners, while others, such as matrix-vector product, do not
- In Computer Science, an object (such as a mesh) that extends another object (such as a vector) is said to *inherit* from the base object.
- Inheritance does not require C++ or Java
- Inheritance helps organize the objects in your library by providing a well-defined taxonomy.
- Lesson 8: Use the principles of object-oriented design to help use hierarchy to structure a library --- use fewer basic concepts to simplify understanding, and use concepts such as inheritance to help (even if your computer language does not directly support it).



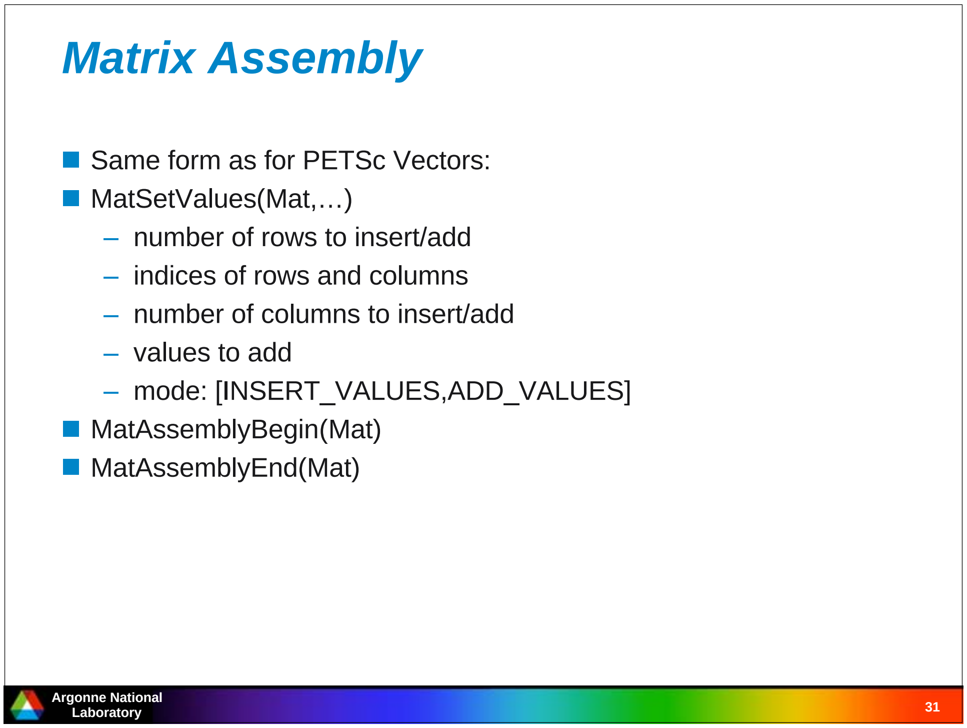
Matrices

- 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.*



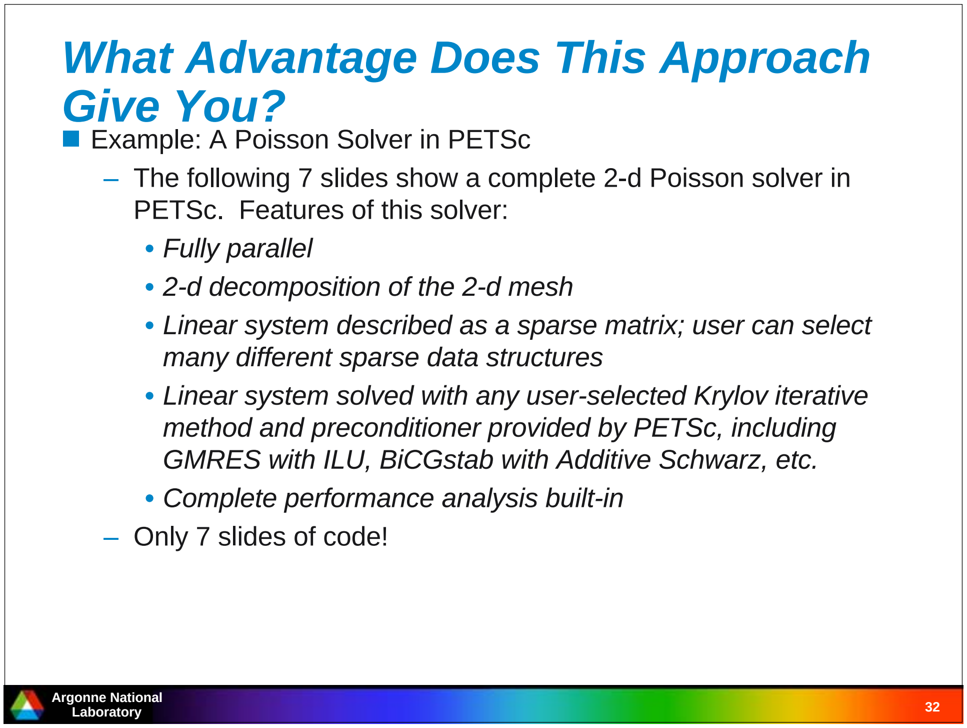
Matrices and Polymorphism

- 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.
- 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



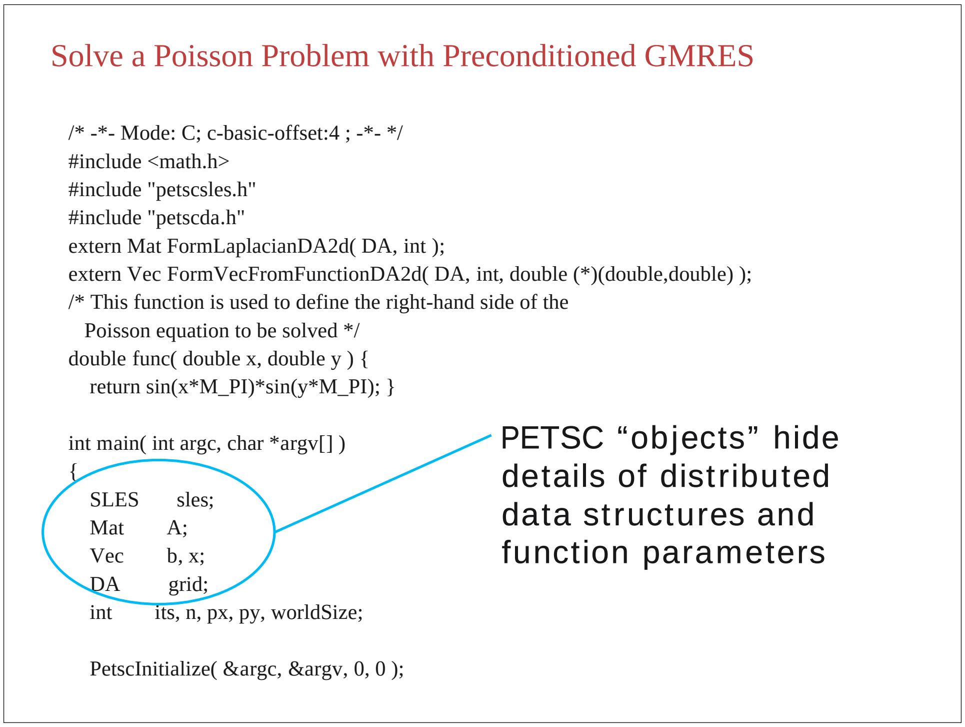
Matrix Assembly

- Same form as for PETSc Vectors:
- 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)



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!



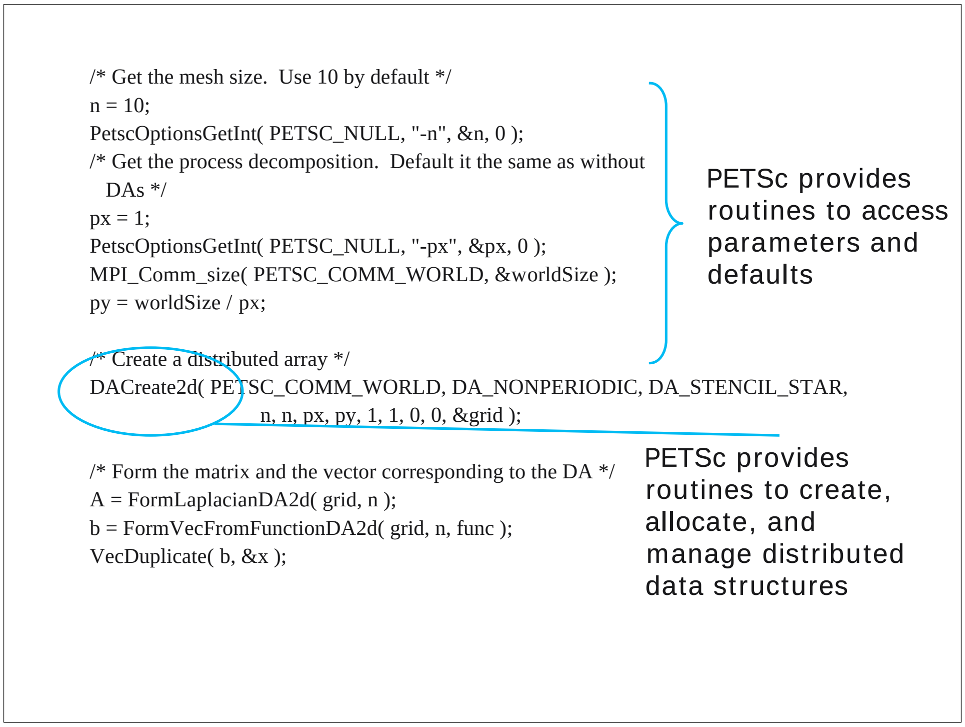
Solve a Poisson Problem with Preconditioned GMRES

```
/* -*- 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



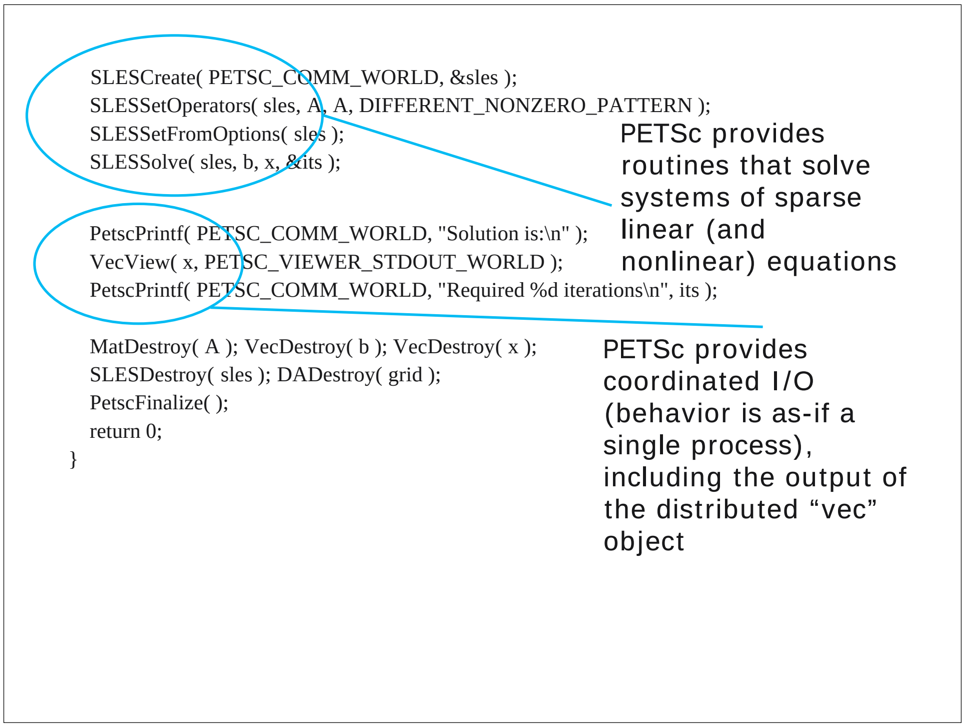
```
/* Get the mesh size.  Use 10 by default */
n = 10;
PetscOptionsGetInt( PETSC_NULL, "-n", &n, 0 );
/* Get the process decomposition.  Default it the same as without
   DAs */
px = 1;
PetscOptionsGetInt( PETSC_NULL, "-px", &px, 0 );
MPI_Comm_size( PETSC_COMM_WORLD, &worldSize );
py = worldSize / px;

/* 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



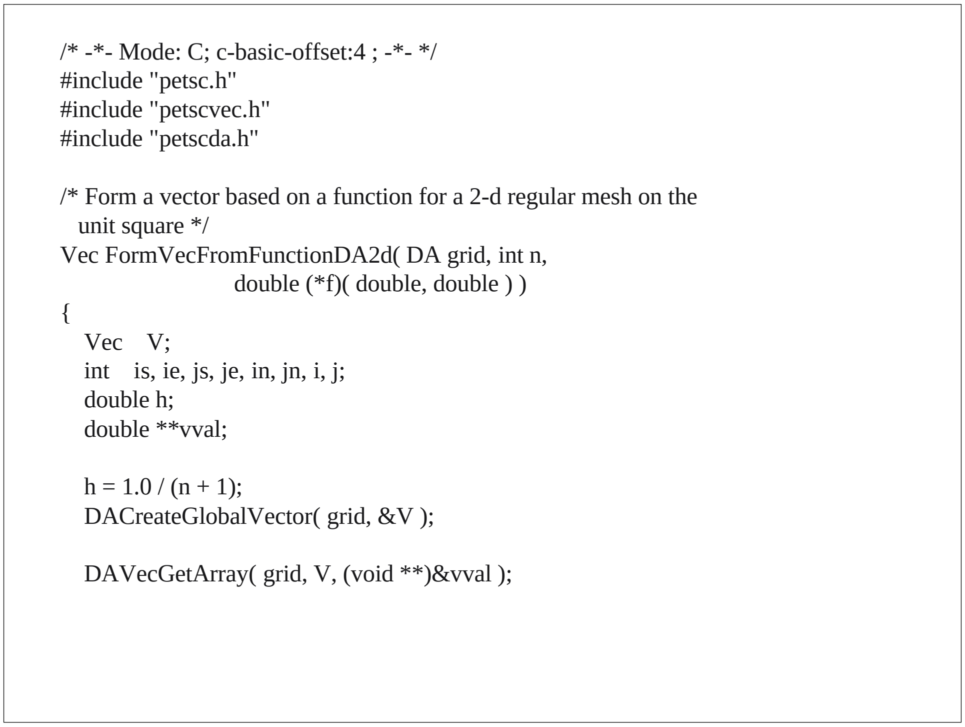
```
    SLESCreate( PETSC_COMM_WORLD, &sles );
    SLESSetOperators( sles, A, A, DIFFERENT_NONZERO_PATTERN );
    SLESSetFromOptions( sles );
    SLESSolve( sles, b, x, &its );

    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

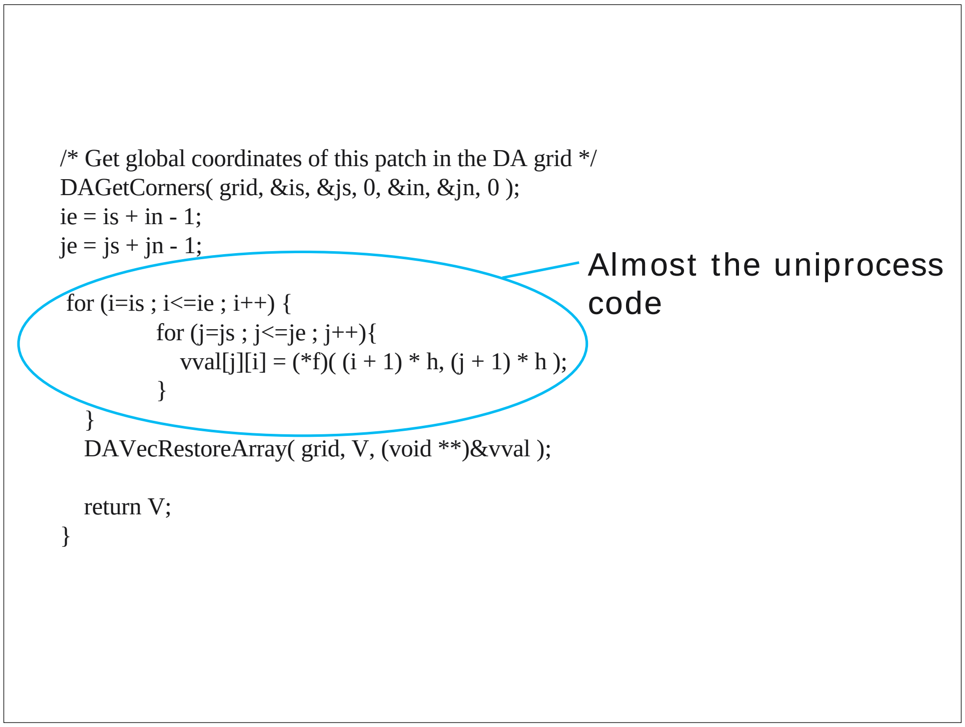


```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
#include "petsc.h"
#include "petscvec.h"
#include "petscda.h"

/* 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 );
```

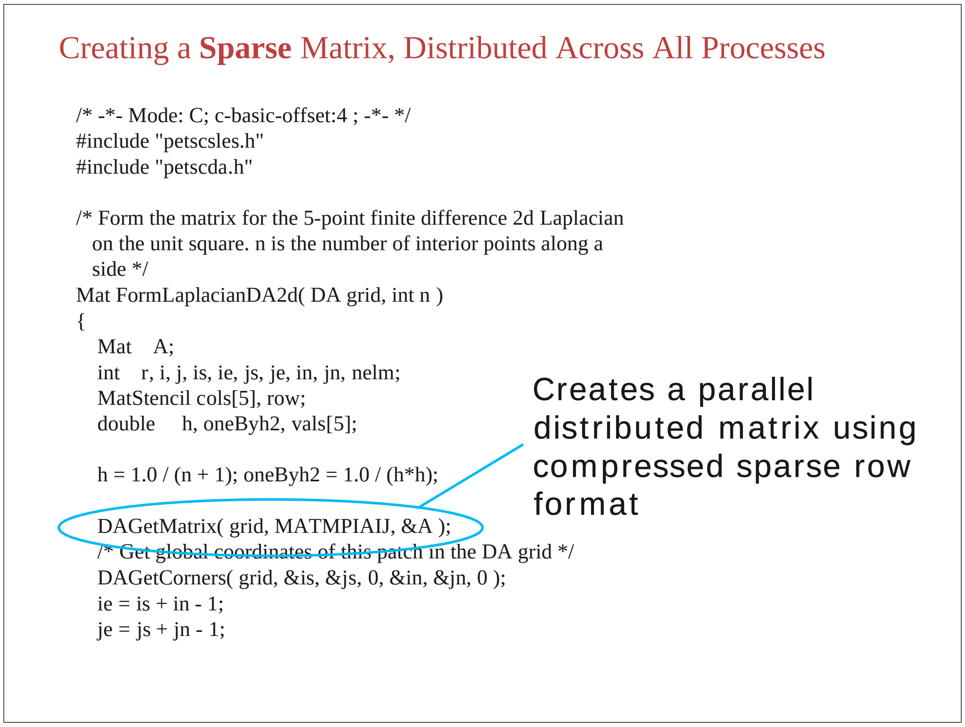


```
/* Get global coordinates of this patch in the DA grid */
DAGetCorners( grid, &is, &js, 0, &in, &jn, 0 );
ie = is + in - 1;
je = js + jn - 1;

 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

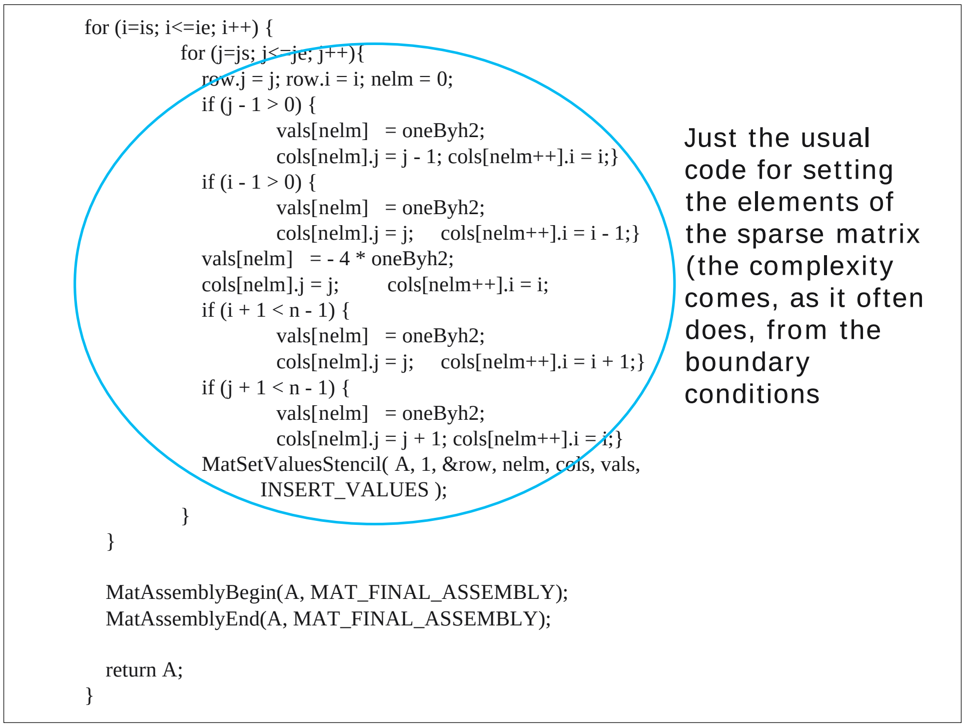
```
/* -*- Mode: C; c-basic-offset:4 ; -*- */
#include "petscsles.h"
#include "petscda.h"

/* 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

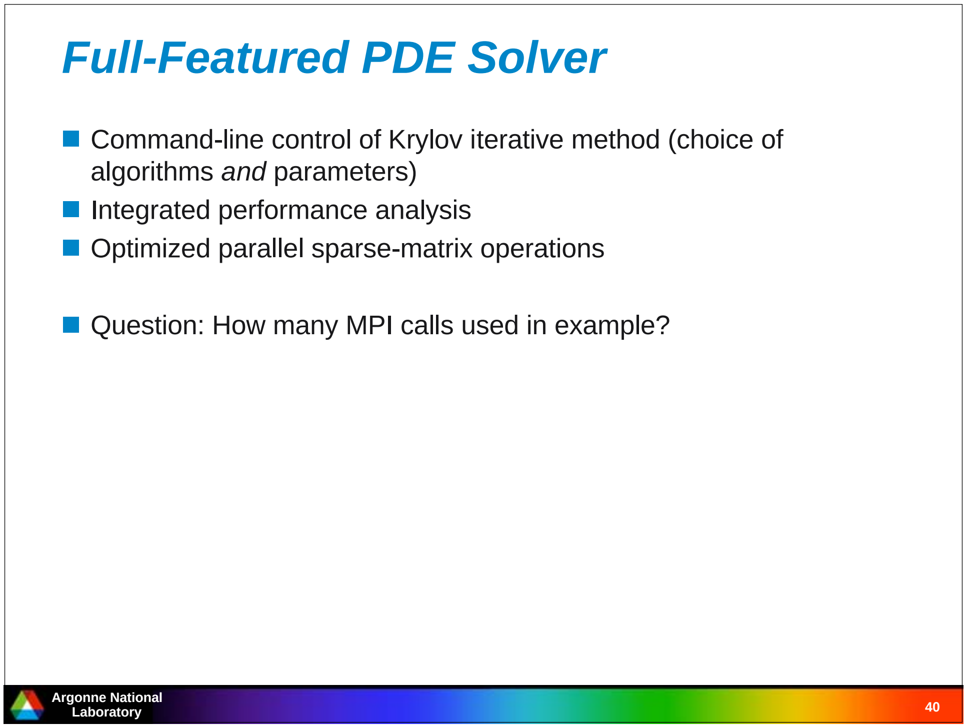


```
for (i=is; i<=ie; i++) {
          for (j=js; j<=je; j++){
            row.j = j; row.i = i; nelm = 0;
            if (j - 1 > 0) {
                    vals[nelm]   = oneByh2;
                    cols[nelm].j = j - 1; cols[nelm++].i = i;}
            if (i - 1 > 0) {
                    vals[nelm]   = 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;
}
```

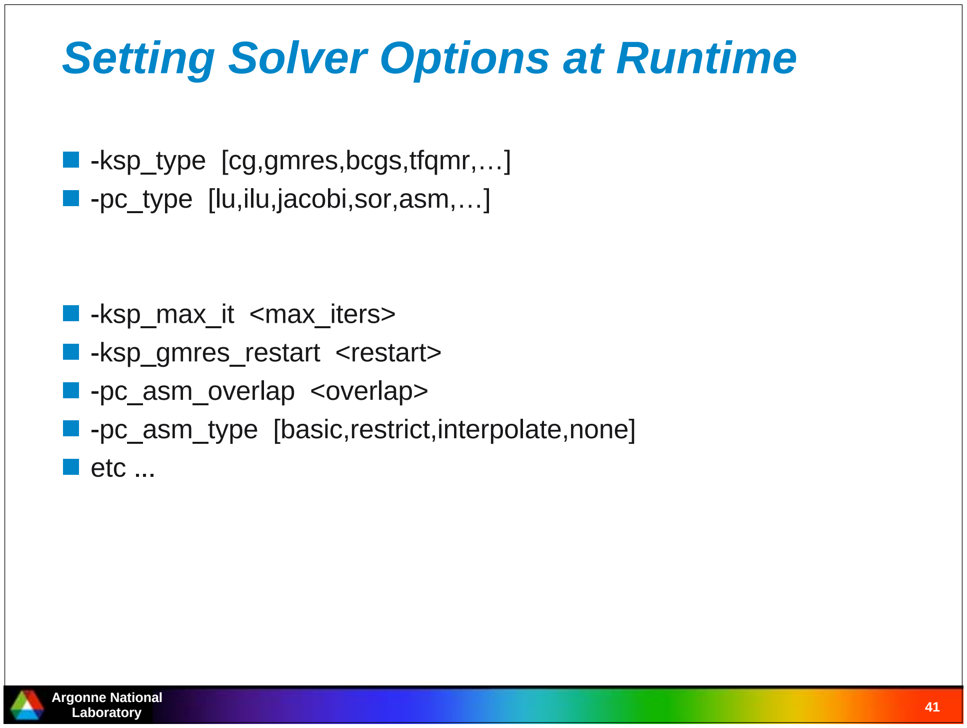
Just the usual code for setting the elements of the sparse matrix (the complexity comes, as it often does, from the boundary conditions



Full-Featured PDE Solver

- Command-line control of Krylov iterative method (choice of algorithms *and* parameters)
- Integrated performance analysis
- Optimized parallel sparse-matrix operations

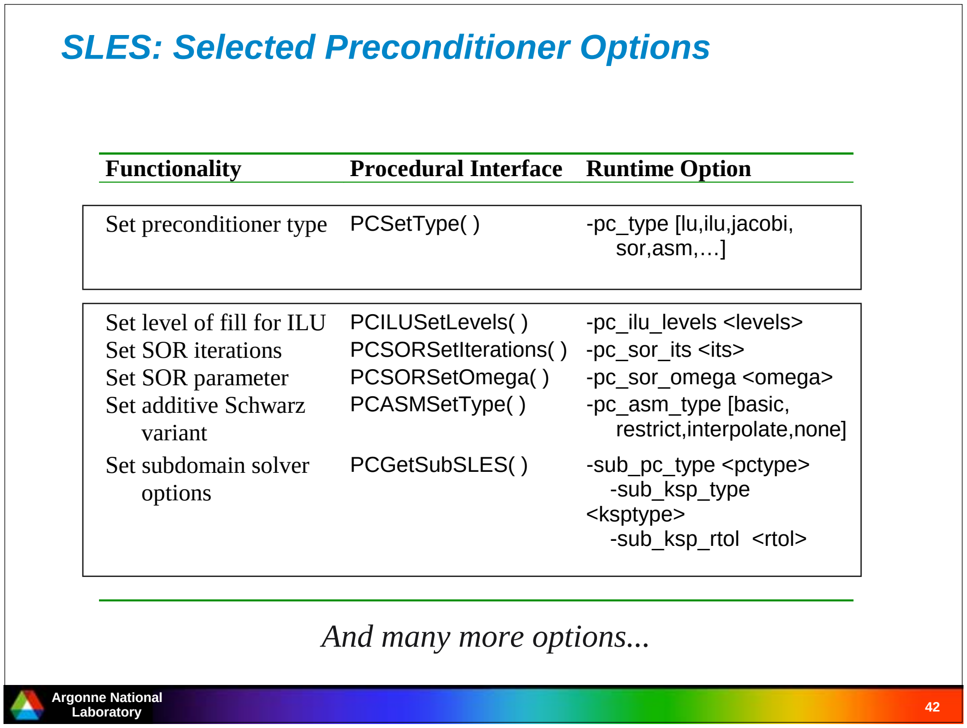
- Question: How many MPI calls used in example?



Setting Solver Options at Runtime

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

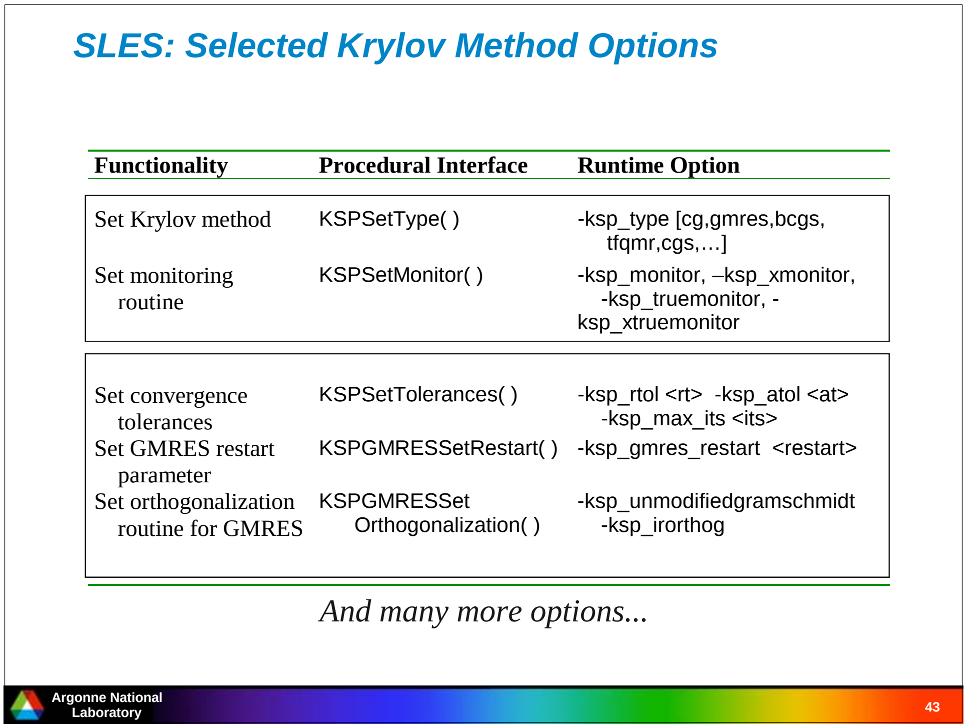
- -ksp_max_it <max_iters>
- -ksp_gmres_restart <restart>
- -pc_asm_overlap <overlap>
- -pc_asm_type [basic,restrict,interpolate,none]
- etc ...



SLES: Selected Preconditioner Options

Functionality	Procedural Interface	Runtime Option
Set preconditioner type	PCSetType( )	-pc_type [lu,ilu,jacobi, sor,asm,…]
Set level of fill for ILU	PCILUSetLevels( )	-pc_ilu_levels <levels>
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	PCGetSubSLES( )	-sub_pc_type <pctype> -sub_ksp_type <ksptype> -sub_ksp_rtol <rtol>

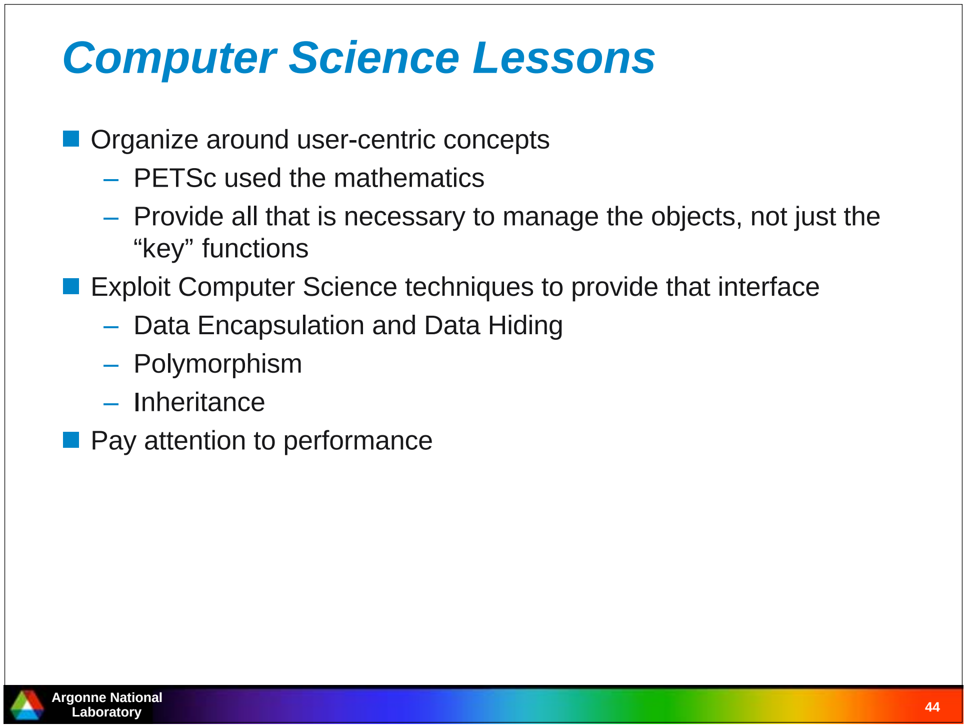
And many more options...



SLES: Selected Krylov Method Options

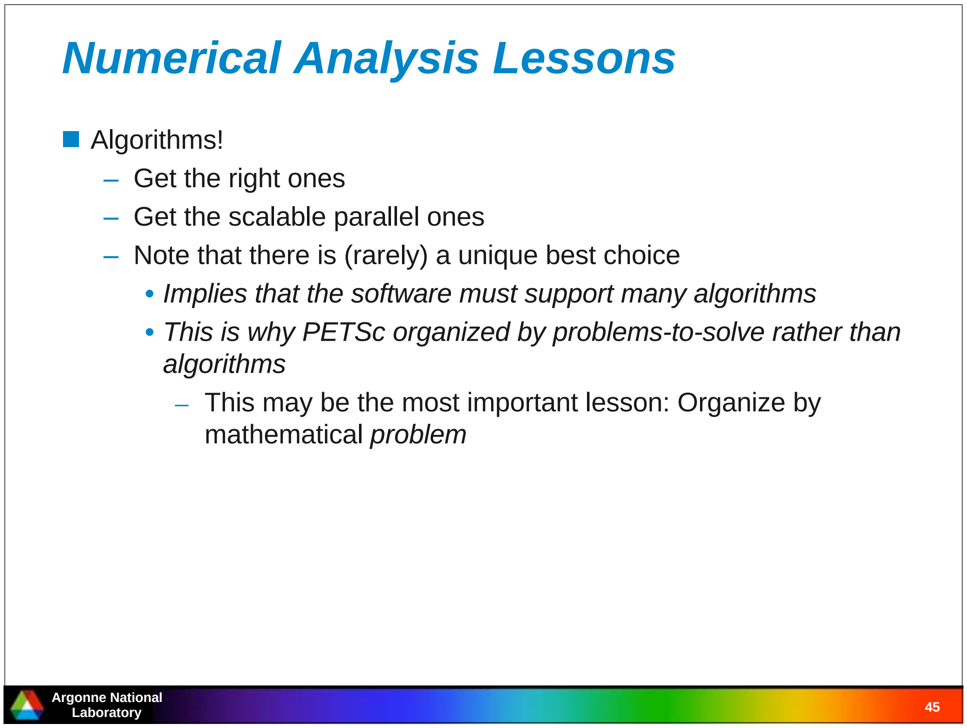
Functionality	Procedural Interface	Runtime Option
Set Krylov method	KSPSetType( )	-ksp_type [cg,gmres,bcgs, tfqmr,cgs,…]
Set monitoring routine	KSPSetMonitor( )	-ksp_monitor, –ksp_xmonitor, -ksp_truemonitor, -ksp_xtruemonitor
Set convergence tolerances	KSPSetTolerances( )	-ksp_rtol <rt> -ksp_atol <at> -ksp_max_its <its>
Set GMRES restart parameter	KSPGMRESSetRestart( )	-ksp_gmres_restart <restart>
Set orthogonalization routine for GMRES	KSPGMRESSet Orthogonalization( )	-ksp_unmodifiedgramschmidt -ksp_irorthog

And many more options...



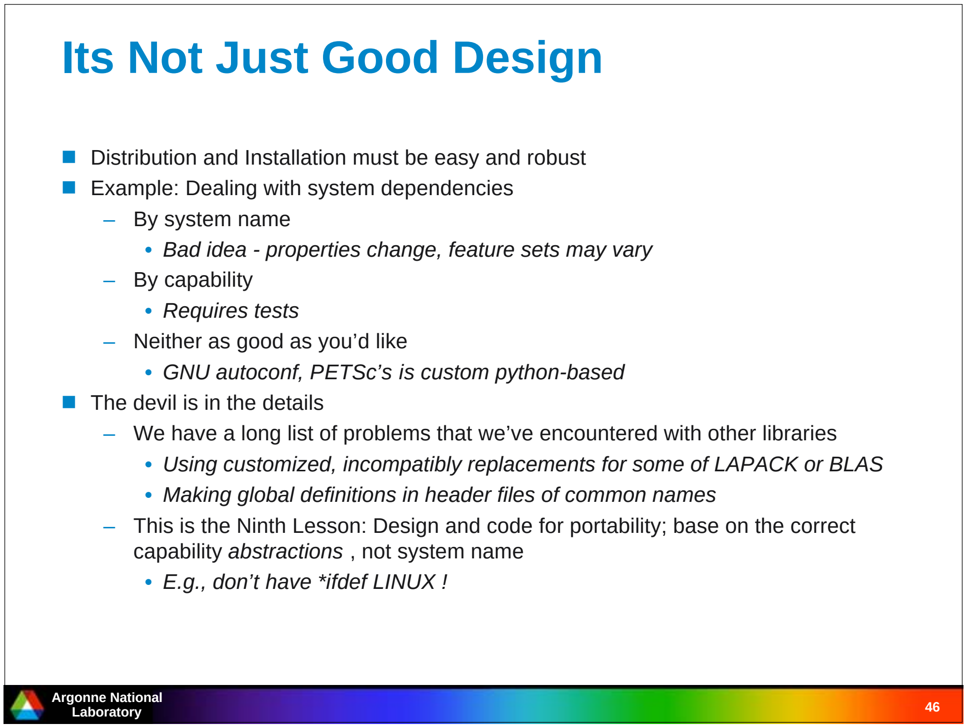
Computer Science Lessons

- 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



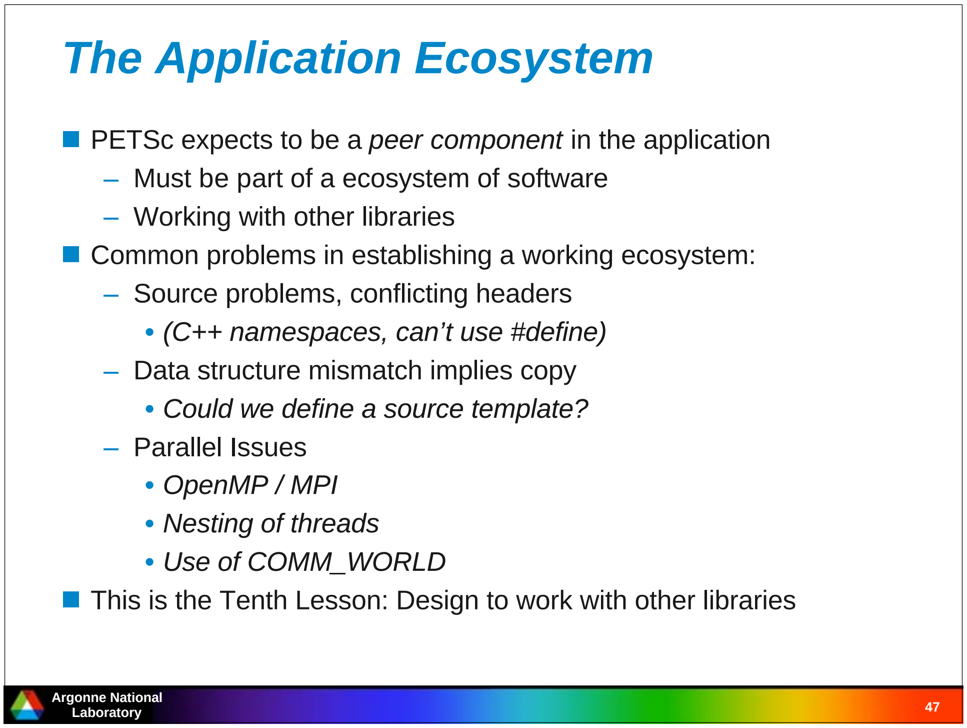
Numerical Analysis Lessons

- 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*



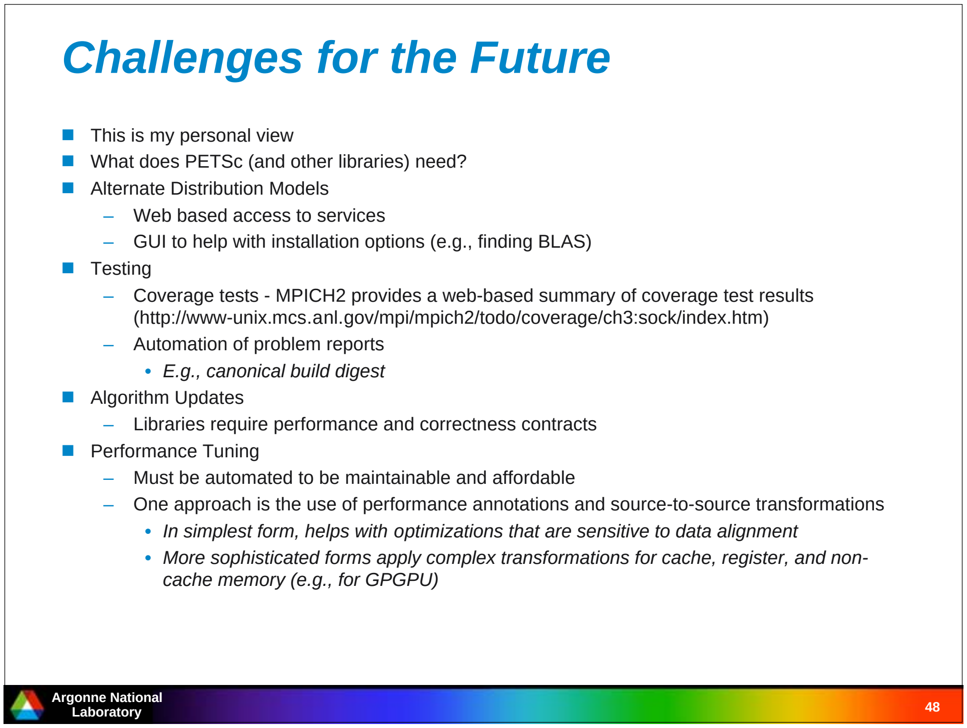
Its Not Just Good Design

- Distribution and Installation must be easy and robust
- Example: Dealing with system dependencies
  - By system name
    - *Bad idea - properties change, feature sets may vary*
  - By capability
    - *Requires tests*
  - Neither as good as you'd like
    - *GNU autoconf, PETSc's is custom python-based*
- The devil is in the details
  - We have a long list of problems that we've encountered with other libraries
    - *Using customized, incompatibly replacements for some of LAPACK or BLAS*
    - *Making global definitions in header files of common names*
  - This is the Ninth Lesson: Design and code for portability; base on the correct capability *abstractions* , not system name
    - *E.g., don't have *ifdef LINUX !*



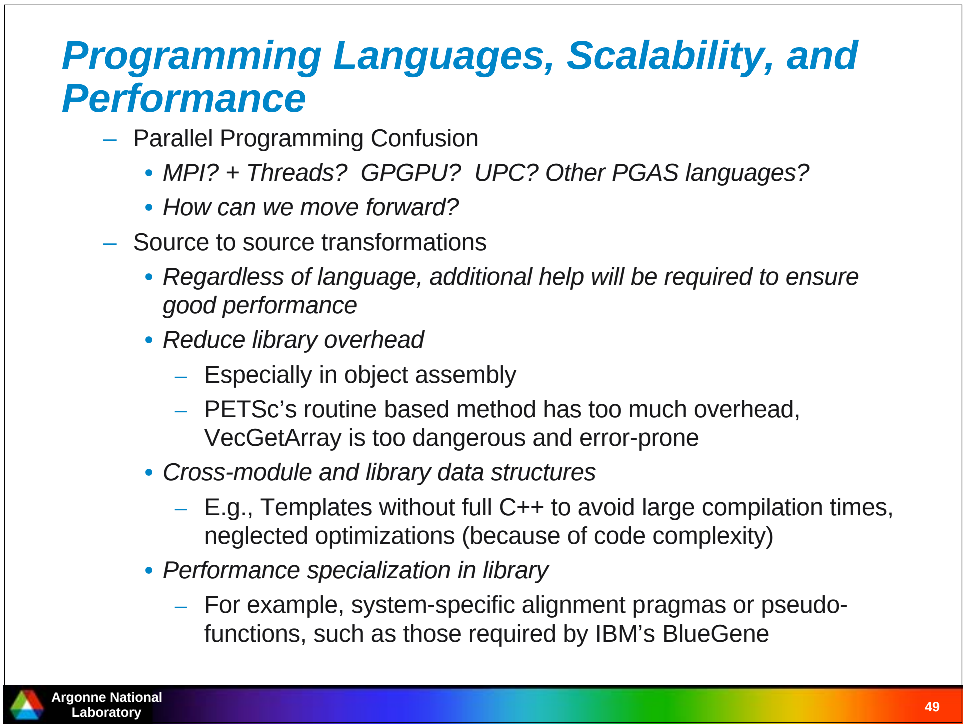
The Application Ecosystem

- PETSc expects to be a *peer component* in the application
  - Must be part of a ecosystem of software
  - Working with other libraries
- Common problems in establishing a working ecosystem:
  - Source problems, conflicting headers
    - *(C++ namespaces, can't use #define)*
  - Data structure mismatch implies copy
    - *Could we define a source template?*
  - Parallel Issues
    - *OpenMP / MPI*
    - *Nesting of threads*
    - *Use of COMM_WORLD*
- This is the Tenth Lesson: Design to work with other libraries



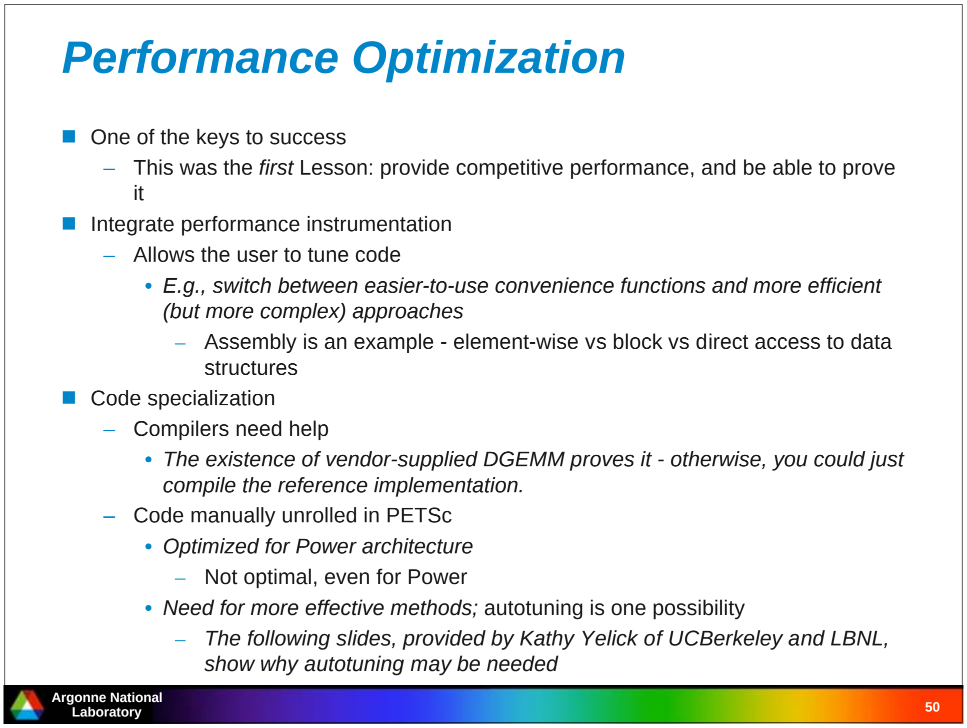
Challenges for the Future

- This is my personal view
- What does PETSc (and other libraries) need?
- Alternate Distribution Models
  - Web based access to services
  - GUI to help with installation options (e.g., finding BLAS)
- Testing
  - Coverage tests - MPICH2 provides a web-based summary of coverage test results (http://www-unix.mcs.anl.gov/mpi/mpich2/todo/coverage/ch3:sock/index.htm)
  - Automation of problem reports
    - *E.g., canonical build digest*
- Algorithm Updates
  - Libraries require performance and correctness contracts
- Performance Tuning
  - Must be automated to be maintainable and affordable
  - One approach is the use of performance annotations and source-to-source transformations
    - *In simplest form, helps with optimizations that are sensitive to data alignment*
    - *More sophisticated forms apply complex transformations for cache, register, and non-cache memory (e.g., for GPGPU)*



Programming Languages, Scalability, and Performance

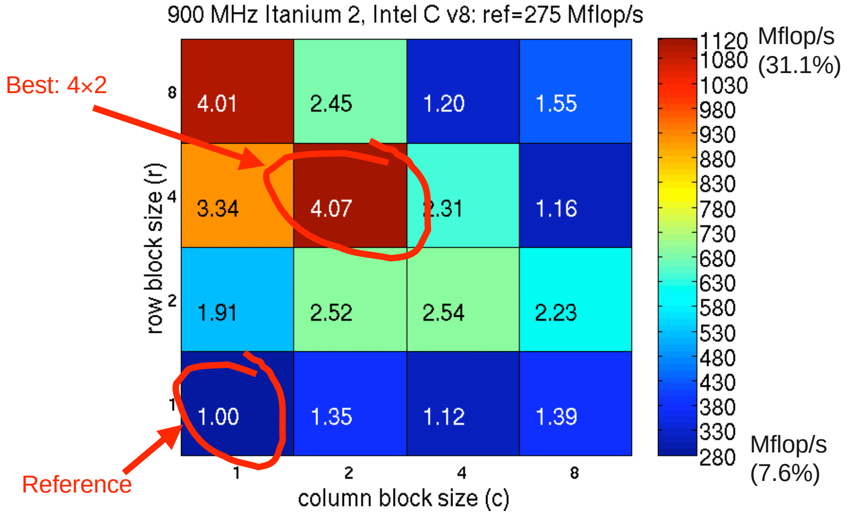
- Parallel Programming Confusion
  - *MPI? + Threads? GPGPU? UPC? Other PGAS languages?*
  - *How can we move forward?*
- Source to source transformations
  - *Regardless of language, additional help will be required to ensure good performance*
  - *Reduce library overhead*
    - Especially in object assembly
    - PETSc’s routine based method has too much overhead, VecGetArray is too dangerous and error-prone
  - *Cross-module and library data structures*
    - E.g., Templates without full C++ to avoid large compilation times, neglected optimizations (because of code complexity)
  - *Performance specialization in library*
    - For example, system-specific alignment pragmas or pseudo-functions, such as those required by IBM’s BlueGene



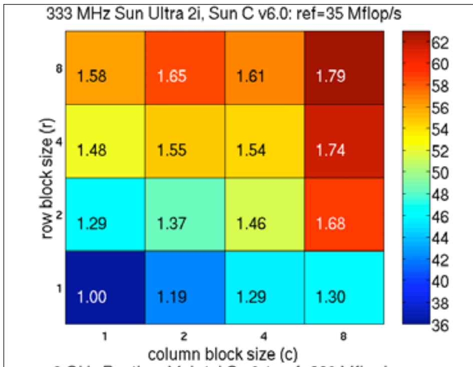
Performance Optimization

- One of the keys to success
  - This was the *first* Lesson: provide competitive performance, and be able to prove it
- Integrate performance instrumentation
  - Allows the user to tune code
    - *E.g., switch between easier-to-use convenience functions and more efficient (but more complex) approaches*
      - Assembly is an example - element-wise vs block vs direct access to data structures
- Code specialization
  - Compilers need help
    - *The existence of vendor-supplied DGEMM proves it - otherwise, you could just compile the reference implementation.*
  - Code manually unrolled in PETSc
    - *Optimized for Power architecture*
      - Not optimal, even for Power
    - *Need for more effective methods;* autotuning is one possibility
      - *The following slides, provided by Kathy Yelick of UCBerkeley and LBNL, show why autotuning may be needed*

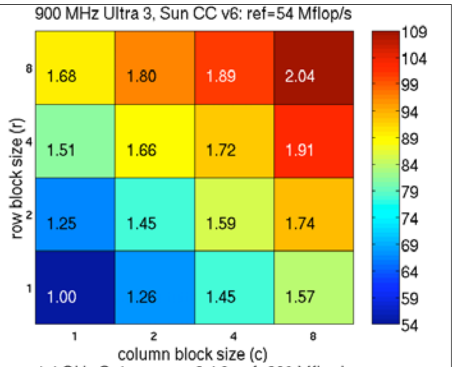
Speedups on Itanium 2: The need for search



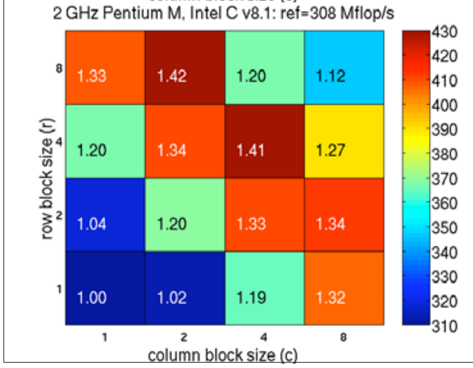
	1	2	4	8
8	4.01	2.45	1.20	1.55
4	3.34	4.07	2.31	1.16
2	1.91	2.52	2.54	2.23
1	1.00	1.35	1.12	1.39



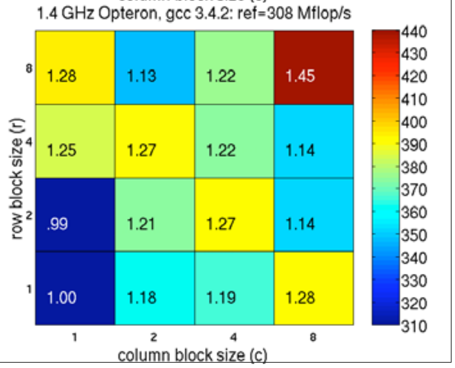
	1	2	4	8
8	1.58	1.65	1.61	1.79
4	1.48	1.55	1.54	1.74
2	1.29	1.37	1.46	1.68
1	1.00	1.19	1.29	1.30



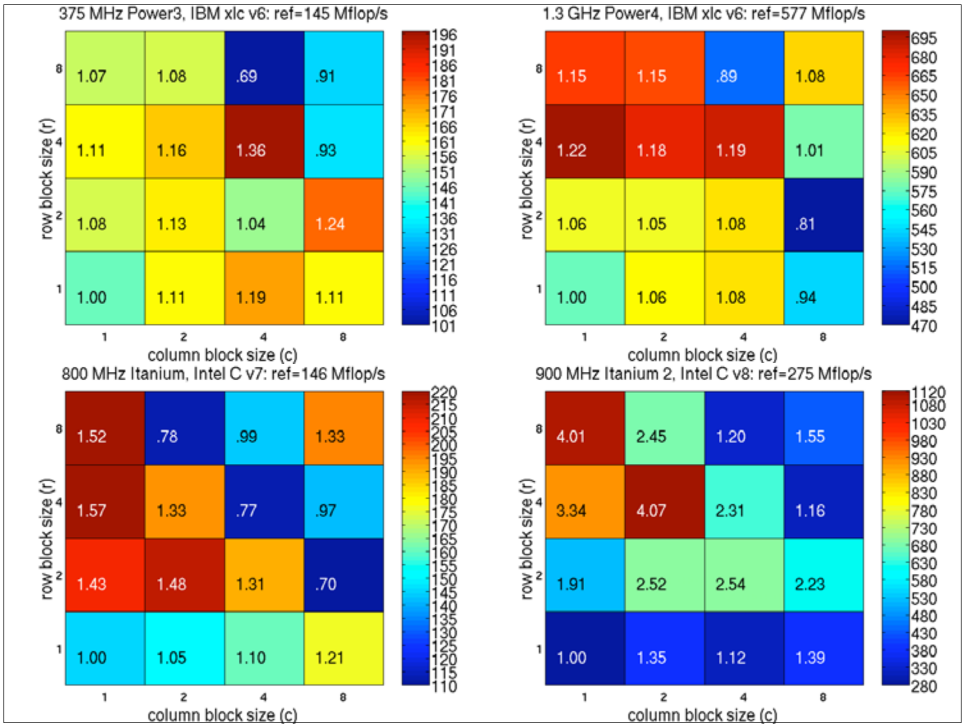
	1	2	4	8
8	1.68	1.80	1.89	2.04
4	1.51	1.66	1.72	1.91
2	1.25	1.45	1.59	1.74
1	1.00	1.26	1.45	1.57



	1	2	4	8
8	1.33	1.42	1.20	1.12
4	1.20	1.34	1.41	1.27
2	1.04	1.20	1.33	1.34
1	1.00	1.02	1.19	1.32

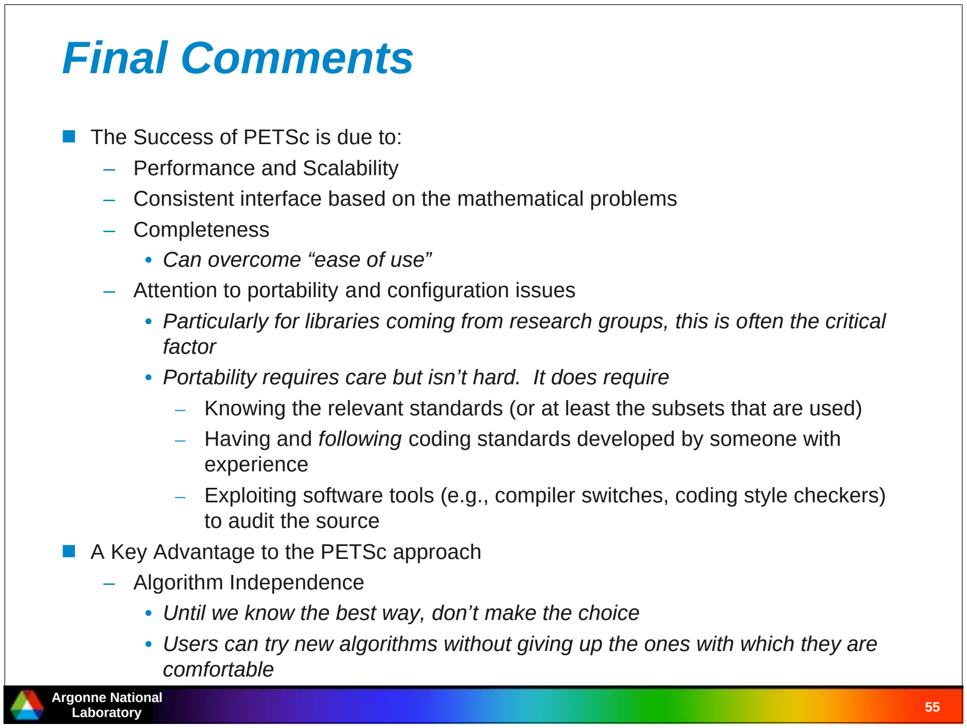


	1	2	4	8
8	1.28	1.13	1.22	1.45
4	1.25	1.27	1.22	1.14
2	.99	1.21	1.27	1.14
1	1.00	1.18	1.19	1.28



Lessons

1. Permit the best performance
2. Provide an escape for customization
3. Define/Update objects as a single operation
4. Provide ease-of-use features, even if they are not high-performance
5. It is good to provide multiple ways to perform the same operation (non-orthogonality of function)
6. Provide special purpose objects (not routines!) for important cases, and then optimize them
7. Allow repeated operations to amortize setup on a per-object basis
8. Use the principles of object oriented design to help use hierarchy to structure a library
9. Design and code for portability; base on the correct capability abstractions, not system name
10. Design to work with other libraries



Final Comments

- The Success of PETSc is due to:
  - Performance and Scalability
  - 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. It does require*
      - Knowing the relevant standards (or at least the subsets that are used)
      - Having and *following* coding standards developed by someone with experience
      - Exploiting software tools (e.g., compiler switches, coding style checkers) to audit the source
- 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*