PETSc Introductory Tutorial

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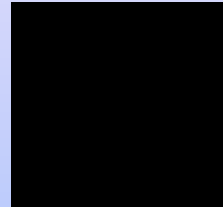June 2006

Presentation Objectives

- Who?
- When?
- Where
- Why?
- What is in PETSc?
- How to use PETSc?

PETSc Development Team

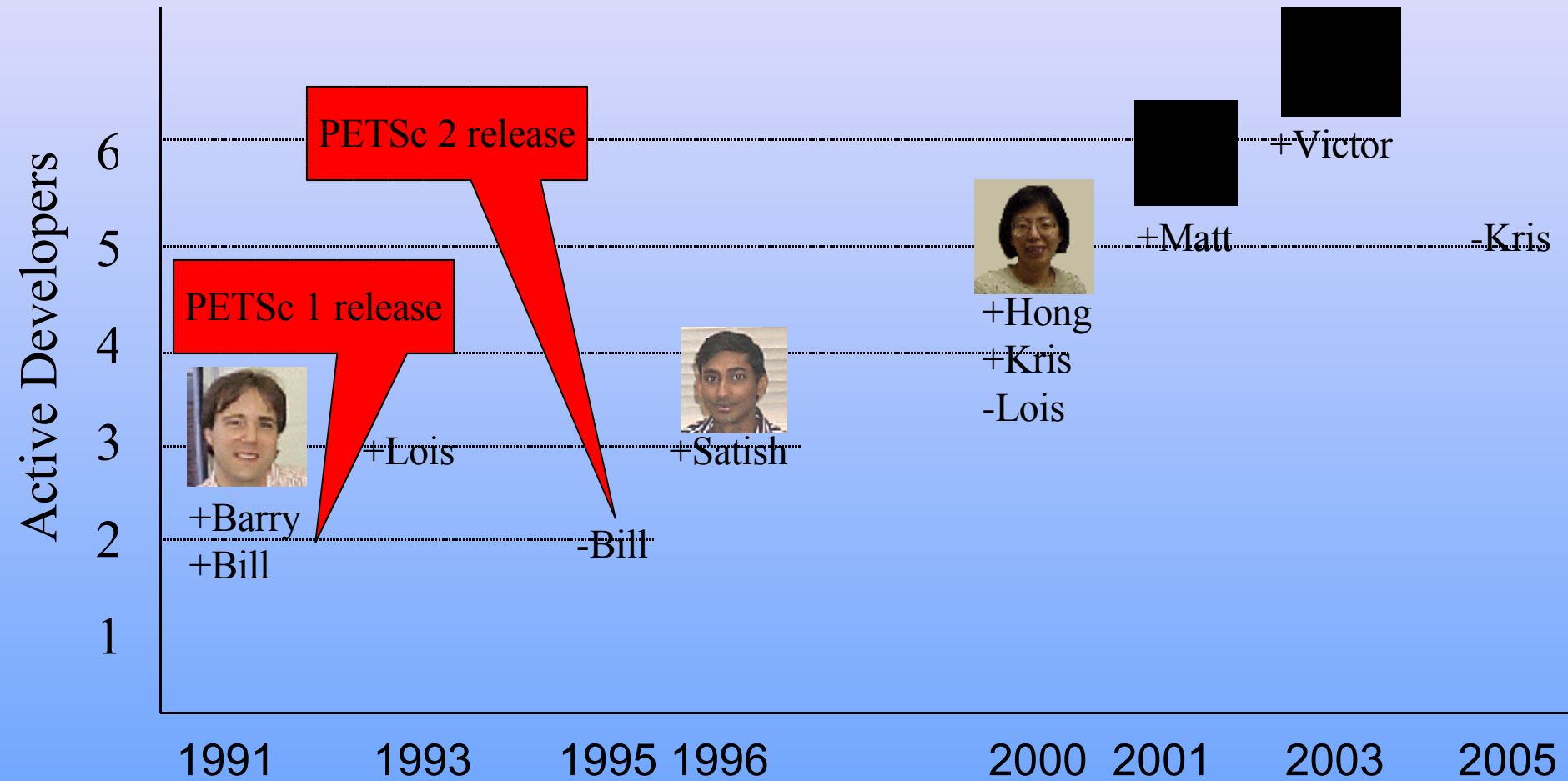Satish Balay

Victor Eijkhout

Matt Knepley

Barry Smith

Hong Zhang

Timeline

Where

Chicago

Argonne: a US Dept of Energy Lab

Why? Original Goals of PETSc

- Provide software for the scalable (parallel) solution of algebraic systems arising from partial differential equation simulations (PDEs).

- Eliminate the MPI from MPI programming

What is PETSc?

- Supported "research" code
  - 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 virtually all systems
    - Cray, SGI, IBM, HP, Sun, Linux, Windows, Apple
- Funded largely by the US Department of Energy

Features

- Support for/uses many numerical packages
- Many (parallel) vector/array operations
- Numerous (parallel) matrix formats
- **Numerous** linear solvers
- Nonlinear solvers
- Limited ODE integrators
- Parallel grid/data management

Support for/uses many numerical packages

- Packages can be automatically
  - downloaded
  - configured and built
  - installed in PETSc

Interfaced Packages

1. LU (Sequential)
   - SuperLU (Demmel and Li, LBNL)
   - ESSL (IBM)
   - Matlab
   - LUSOL (from MINOS - Michael Saunders, Stanford)
   - LAPACK
   - PLAPACK (van de Geijn, UT Austin)
   - UMFPACK (Timothy A. Davis)
- Parallel LU
   - SuperLU_dist (Demmel and Li, LBNL)
   - SPOOLES (Ashcroft, Boeing, funded by ARPA)
   - MUMPS (European)
   - PLAPACK (van de Geijn, UT Austin)
- Parallel Cholesky –
   - DSCPACK (Raghavan, Penn. State)
   - SPOOLES (Ashcroft, Boeing, funded by ARPA)
   - PLAPACK (van de Geijn, UT Austin)

Interfaced Packages

1. XYTlib – parallel direct solver (Fischer and Tufo, ANL)
2. SPAI – Sparse approximate inverse (parallel)
    - Parasails (Chow, part of Hypre, LLNL)
    - SPAI 3.0 (Grote/Barnard)
3. Algebraic multigrid
    - Parallel BoomerAMG (part of Hypre, LLNL)
    - ML (part of Trilinos, SNL)
4. Parallel ICC(0) – BlockSolve95 (Jones and Plassman, ANL)
5. Parallel ILU
    - BlockSolve95 (Jones and Plassman, ANL)
    - PILUT (part of Hypre, LLNL)
    - EUCLID (Hysom – also part of Hypre, ODU/LLNL)
6. Sequential ILUDT (SPARSEKIT2- Y. Saad, U of MN)

Interfaced Packages

1. Parititioning
   - Parmetis
   - Chaco
   - Jostle
   - Party
   - Scotch
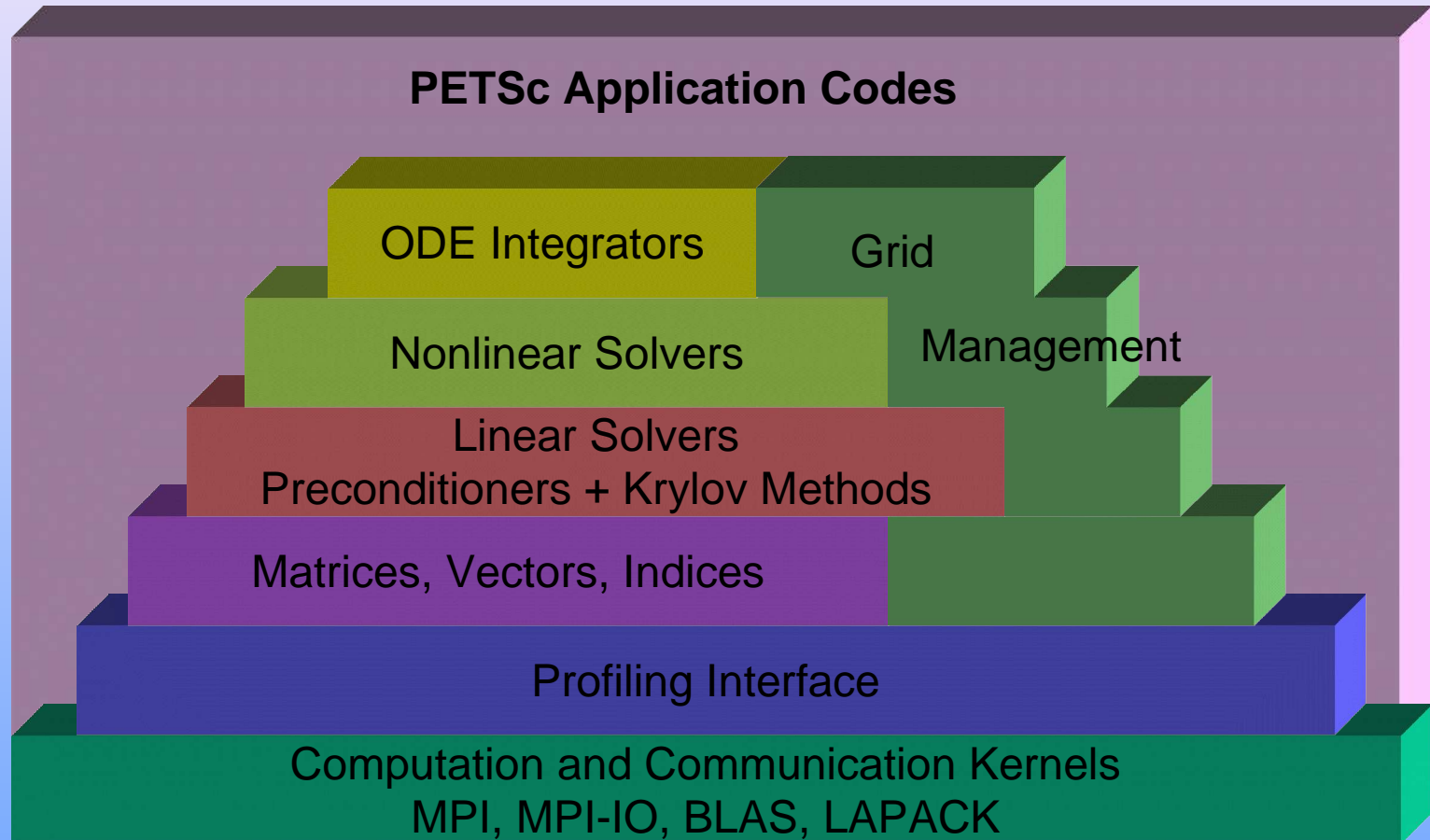- ODE integrators
   - Sundials (LLNL)
12. Eigenvalue solvers
   - BLOPEX (developed by Andrew Knyazev)

Size Limitations?

- PETSc has done problem with 500 million unknowns
  http://www.scconference.org/sc2004/schedule/pdfs/pap111.pdf

- PETSC has used on over 6,000 processors
  ftp://info.mcs.anl.gov/pub/tech_reports/reports/P776.ps.Z

- PETSC applications have run at two tera-flops

Structure of PETSc

PETSc Application Codes

ODE Integrators

Grid

Nonlinear Solvers

Management

Linear Solvers
Preconditioners + Krylov Methods

Matrices, Vectors, Indices

Profiling Interface

Computation and Communication Kernels
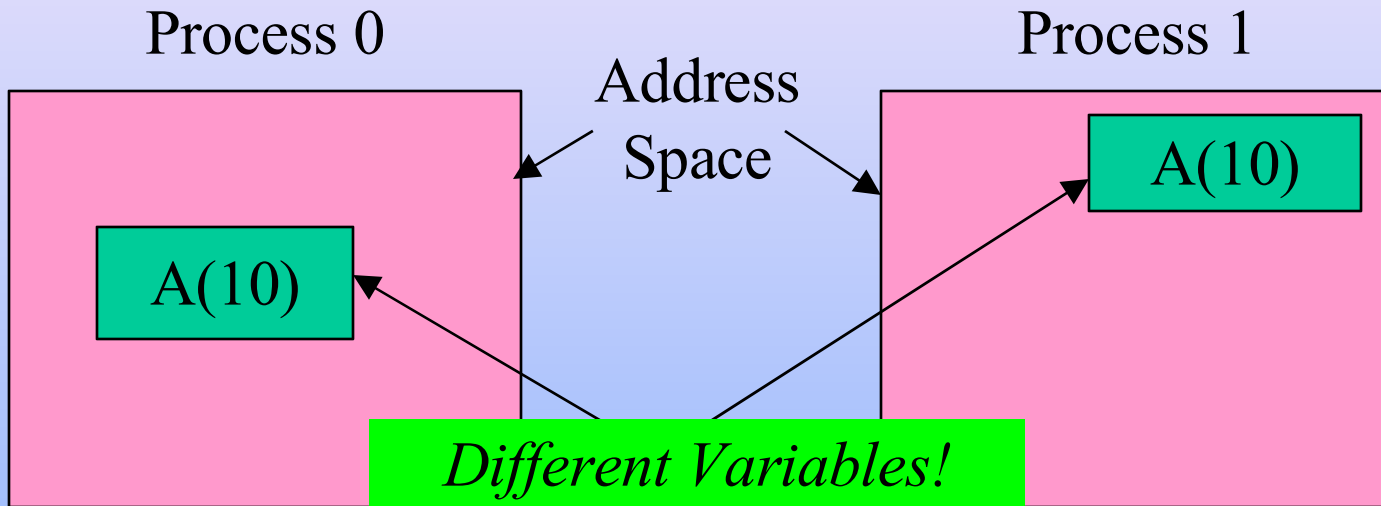MPI, MPI-IO, BLAS, LAPACK

PETSc Structure

Object Oriented Programming

Design based not on the data in object, but instead based on operations you perform with or on the data

For example a vector is not a 1d array of numbers but an abstract object where addition and scalar multiplication (and likely many more) are defined

PETSc Structure

The PETSc Programming Model

- Distributed memory, "shared-nothing"
  - Requires only a standard compiler
  - Access to data on remote machines through MPI
- Hide within objects the details of the communication
- User orchestrates communication at a higher abstract level then direct MPI calls

PETSc Structure

Distributed Memory Model

Process 0

Process 1

Address Space

A(10)

A(10)

Different Variables!

- Integer A(10)

    …

    print *, A

- Integer A(10)
  do i=1,10
    A(i) = i
  enddo
  ...

This A is completely different from this one

Collectivity

- MPI communicators (MPI_Comm) specify collectivity

  – Processes involved in a computation

- PETSc constructors are collective over a communicator

  – VecCreate(MPI_Comm comm, int m, int M, Vec *x)

  – Use **PETSC_COMM_WORLD** for all processes

- Some operations are collective, while others are not

  – collective: VecNorm()

  – not collective: VecGetLocalSize()

- If a sequence of collective routines is used, they **must** be called in the same order by each process.

What is not in PETSc?

- Higher level representations of mathematical objects
- Operator overloading
- Automatic load balancing
- Sophisticated visualization capabilities
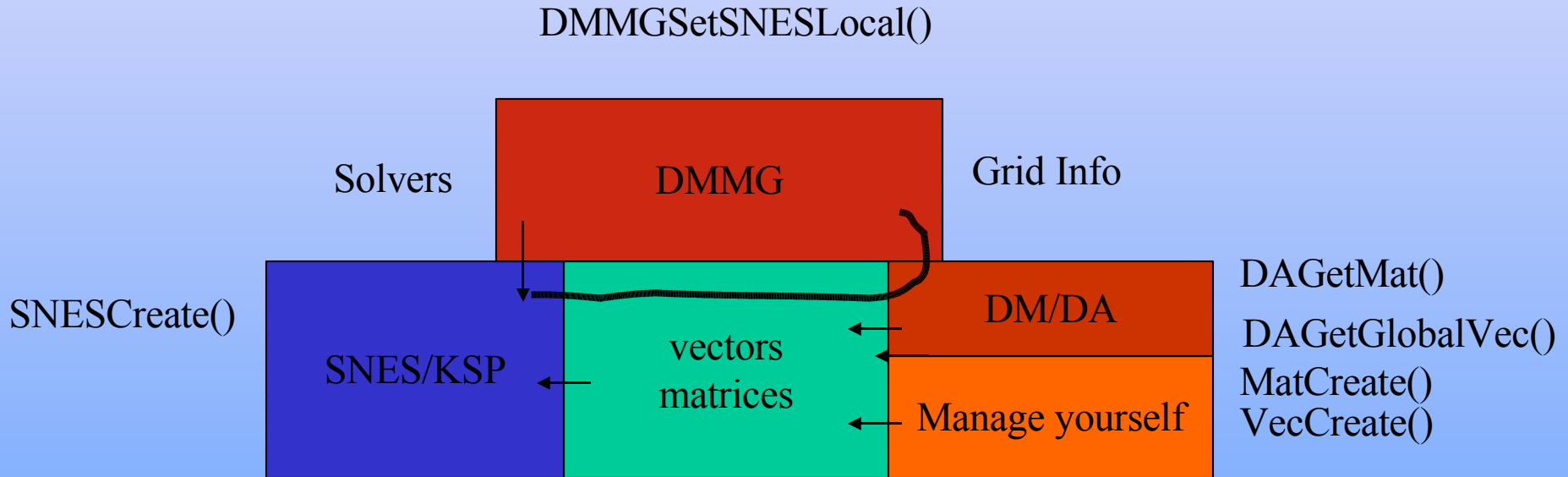- Optimization and sensitivity, BUT

PETSc Structure

Child Packages of PETSc

- SIPs - Shift-and-Invert Parallel Spectral Transformations

- SLEPc - scalable eigenvalue/eigenvector solver packages.

- TAO - scalable optimization algorithms

All have PETSc's style of programming

PETSc is only a Library

- PETSc is merely a set of library interfaces
  - We do not seize main()
  - We do not control output
  - We propagate errors from underlying packages
  - We present (largely) the same interfaces in:
    - C
    - C++
    - F77
    - F90

See Gropp in SIAM, OO Methods for Interop SciEng, '99

Integration

Three Ways of Using PETSc

DMMGSetSNESLocal()

Solvers   DMMG   Grid Info

SNESCreate()

SNES/KSP

vectors matrices

DM/DA

Manage yourself

DAGetMat()
DAGetGlobalVec()
MatCreate()
VecCreate()

Getting Started

- Call PetscInitialize()

  – Sets up static data and services

  – Sets up MPI if it is not already

- Call PetscFinalize()

  – Calculates logging summary

  – Shuts down and release resources

Integration

Getting Started

```
PetscInitialize(&argc,&argv,(char*)0,help);
…
PetscFinalize();

return 0;


Call PetscInitialize(PETSC_NULL_CHARACTER)
…
call PetscFinalize(ierr)
end
```

Integration

Linear Algebra I

- Vectors
  - Has a direct interface to the values
  - Supports all vector space operations
    - VecDot(), VecNorm(), VecScale()
  - Also unusual ops, e.g. VecSqrt()
  - Automatic communication during assembly
  - Customizable communication (scatters)

Integration

PETSc Numerical Components

Nonlinear Solvers		
Newton-based Methods		Other
Line Search	Trust Region	

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	LU (Sequential only)	Others

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

Distributed Arrays

Index Sets			
Indices	Block Indices	Stride	Other

Vectors

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(MPI_Comm,Vec *)
    - MPI_Comm - processes that share the vector
  - VecSetSizes(Vec, int, int)
    - number of elements local to this process
    - or total number of elements
  - VecSetType(Vec,VecType)
    - Where VecType is
      - VEC_SEQ, VEC_MPI, or VEC_SHARED
    - VecSetFromOptions(Vec) lets you set the type at *runtime*

proc 0

proc 1

proc 2

proc 3

proc 4
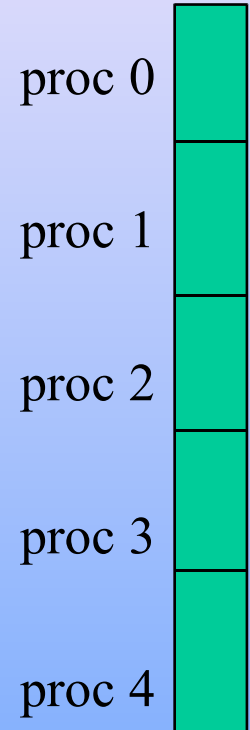
data objects:
vectors

Creating a vector

Vec x;
int N;
…
PetscInitialize(&argc,&argv,(char*)0,help);
PetscOptionsGetInt(PETSC_NULL,"-n",&N,PETSC_NULL);
…
VecCreate(PETSC_COMM_WORLD,&x);
VecSetSizes(x,PETSC_DECIDE,N);
VecSetType(x,VEC_MPI);
VecSetFromOptions(x);

Use PETSc to get value
from command line

Global size

PETSc determines
local size

data objects:
vectors

How Can We Use a PETSc Vector

- PETSc supports "data structure-neutral" objects
  - distributed memory "shared nothing" model
  - single processors and shared memory systems
- PETSc vector is a "handle" to the real vector
  - Allows the vector to be distributed across many processes
  - To access the *elements* of the vector, we cannot simply do
      for (i=0; i<N; i++) v[i] = i;
  - We do not *require* that the programmer work only with the "local" part of the vector; we permit operations, such as setting an element of a vector, to be performed globally
- Recall how data is stored in the distributed   memory programming model…

data objects: vectors

Vector Assembly

- A three step process
  - Each process tells PETSc what values to set or add to a vector component. Once *all* values provided,
  - Begin communication between processes to ensure that values end up where needed
  - (allow other operations, such as some computation, to proceed)
  - Complete the communication
- VecSetValues(Vec,…)
  - number of entries to insert/add
  - indices of entries
  - values to add
  - mode: [INSERT_VALUES,ADD_VALUES]
- VecAssemblyBegin(Vec)
- VecAssemblyEnd(Vec)

data objects:
vectors

Parallel Matrix and Vector Assembly

- Processes may generate any entries in vectors and matrices

- Entries need not be generated on the process on which they ultimately will be stored

- **PETSc automatically moves data during the assembly process if necessary**

data objects:
vectors

One Way to Set the Elements of A Vector

```
VecGetSize(x,&N);  /* Global size */
MPI_Comm_rank(PETSC_COMM_WORLD, &rank);
if (rank == 0) {
    for (i=0; i<N; i++)                    VecSetValues
(x,1,&i,&i,INSERT_VALUES);
}
```

Vector index

Vector value

```
/* These two routines ensure that the data is
distributed to the other processes */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
```

data objects:
vectors

A Parallel Way to Set the Elements of A Distributed Vector

```
VecGetOwnershipRange(x,&low,&high);
for (i=low; i<high; i++)
VecSetValues(x,1,&i,&i,INSERT_VALUES);


/* These two routines must be called (in case
some other process contributed a value owned by
another process) */
VecAssemblyBegin(x);
VecAssemblyEnd(x);
```

data objects:
vectors

Selected Vector Operations

Function Name	Operation
VecAXPY(Scalar *a, Vec x, Vec y)	$y = y + a*x$
VecAYPX(Scalar *a, Vec x, Vec y)	$y = x + a*y$
VecWAXPY(Scalar *a, Vec x, Vec y, Vec w)	$w = a*x + y$
VecScale(Scalar *a, Vec x)	$x = a*x$
VecCopy(Vec x, Vec y)	$y = x$
VecPointwiseMult(Vec x, Vec y, Vec w)	$w\_i = x\_i *y\_i$
VecMax(Vec x, int *idx, double *r)	$r = max\ x\_i$
VecShift(Scalar *s, Vec x)	$x\_i = s + x\_i$
VecAbs(Vec x)	$x\_i = |x\_i|$
VecNorm(Vec x, NormType type , double *r)	$r = ||x||$

data objects:
vectors

A Complete PETSc Program

```c
#include petscvec.h
int main(int argc,char **argv)
{
  Vec x;
  int n = 20,ierr;
  PetscTruth flg;
  PetscScalar one = 1.0, dot;


  PetscInitialize(&argc,&argv,0,0);
  PetscOptionsGetInt(PETSC_NULL,"-n",&n,PETSC_NULL);
  VecCreate(PETSC_COMM_WORLD,&x);
  VecSetSizes(x,PETSC_DECIDE,n);
  VecSetFromOptions(x);
  VecSet(&one,x);
  VecDot(x,x,&dot);
  PetscPrintf(PETSC_COMM_WORLD,"Vector length %dn",(int)dot);
  VecDestroy(x);
  PetscFinalize();
  return 0;
}
```

data objects:
vectors

Working With Local Vectors

- It is sometimes more efficient to directly access the storage for the local part of a PETSc Vec.
  - E.g., for finite difference computations involving elements of the vector

- PETSc allows you to access the local storage with
  - VecGetArray(Vec, double *[ ])
- You must return the array to PETSc when you finish
  - VecRestoreArray(Vec, double *[ ])

- Allows PETSc to handle data structure conversions
  - For most common uses, these routines are inexpensive and do *not* involve a copy of the vector.

data objects:
vectors

Example of VecGetArray

Vec   vec;

Double *avec;

…

VecCreate(PETSC_COMM_SELF,&vec);
VecSetSizes(vec,PETSC_DECIDE,N);
VecSetFromOptions(vec);

VecGetArray(vec,&avec);
/* compute with avec directly, e.g., */

PetscPrintf(PETSC_COMM_WORLD,
 "First element of local array of vec in each process is %f\n",
avec[0]);
VecRestoreArray(vec,&avec);

data objects:
vectors

Indexing

- Non-trivial in parallel
- PETSc IS object, generalization of
  - {0,3,56,9}
  - 1:4:55
  - Indexing by block

Linear Algebra II

- Matrices
  - Must use MatSetValues()
    - Automatic communication
  - Supports many data types
    - AIJ, Block AIJ, Symmetric AIJ, Block Diagonal, etc.
  - Supports structures for many packages
    - Spooles, MUMPS, SuperLU, UMFPack, DSCPack

Integration

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*.

data objects: matrices

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.

- A matrix is defined by its *interface*, the operations that you can perform with it.
  - Not by its data structure

data objects:
matrices

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)

data objects:
matrices

Matrix Assembly Example

simple 3-point stencil for 1D discretization

```
Mat        A;
int        column[3], i;
double value[3];
…
MatCreate(PETSC_COMM_WORLD,&A);
MatSetSizes(A,PETSC_DECIDE,PETSC_DECIDE,N,N);
MatSetFromOptions(A);
/* mesh interior */
value[0] = -1.0; value[1] = 2.0; value[2] = -1.0;
if (rank == 0) {  /* Only one process creates matrix entries */
   for (i=1; i<N-2; 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  (code for global row 0 and N-1 omitted) */
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```
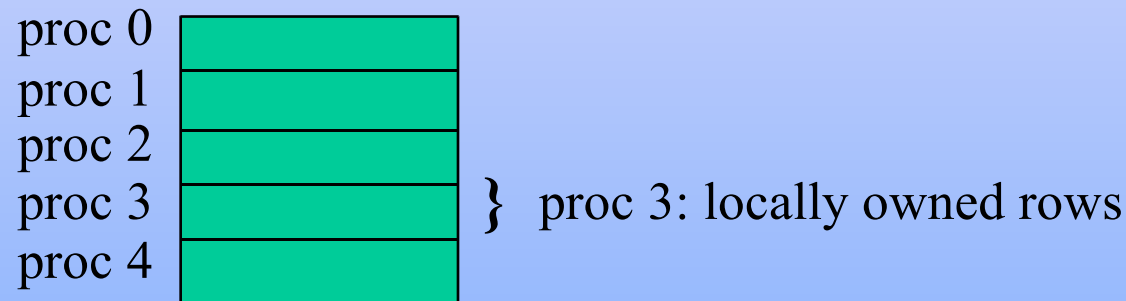
Choose the global size of the matrix

Let PETSc decide how to allocate matrix across processes

data objects: matrices

Parallel Matrix Distribution

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

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

MatGetOwnershipRange(Mat A, int *rstart, int *rend)

- rstart: first locally owned row of global matrix

- rend -1: last locally owned row of global matrix

data objects:
matrices

Matrix Assembly Example With Parallel Assembly

simple 3-point stencil for 1D discretization

```
Mat      A;
int      column[3], i, start, end,istart,iend;
double value[3];
…
MatCreate(PETSC_COMM_WORLD,&A);
MatSetSizes(A,PETSC_DECIDE,PETSC_DECIDE,N,N);
MatSetFromOptions(A);
MatGetOwnershipRange(A,&start,&end);
/* mesh interior */
istart = start; if (start == 0) istart = 1;
iend = end; if (iend == n-1) iend = n-2;
value[0] = -1.0; value[1] = 2.0; value[2] = -1.0;
for (i=istart; i<iend; i++) { /* each processor generates some of the matrix values */
    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  (code for global row 0 and n-1 omitted) */
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```
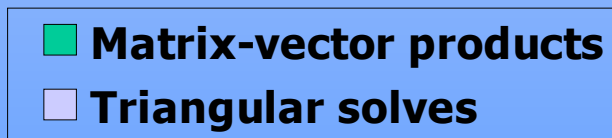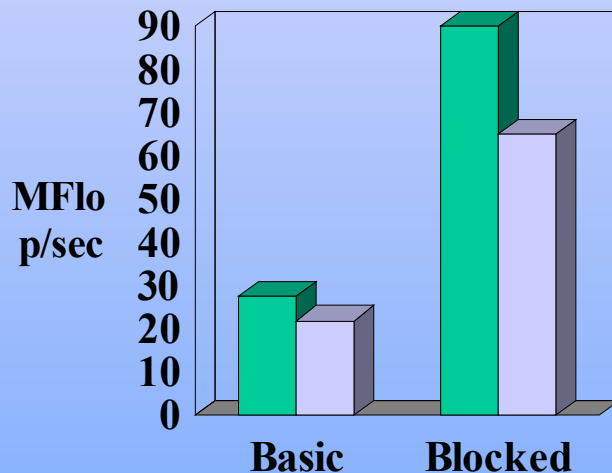
data objects:
matrices

Why Are PETSc Matrices The Way They Are?

- No one data structure is appropriate for all problems
  - Blocked and diagonal formats provide significant performance benefits
  - PETSc provides a large selection of formats and makes it (relatively) easy to extend PETSc by adding new data structures
- Matrix assembly is difficult enough without being forced to worry about data partitioning
  - PETSc provides parallel assembly routines
  - Achieving high performance still requires making most operations local to a process but programs can be incrementally developed.
- Matrix decomposition by consecutive rows across processes, **for sparse matrices**, is simple and makes it easier to work with other codes.
  - For applications with other ordering needs, PETSc provides "Application Orderings" (AO), described later.

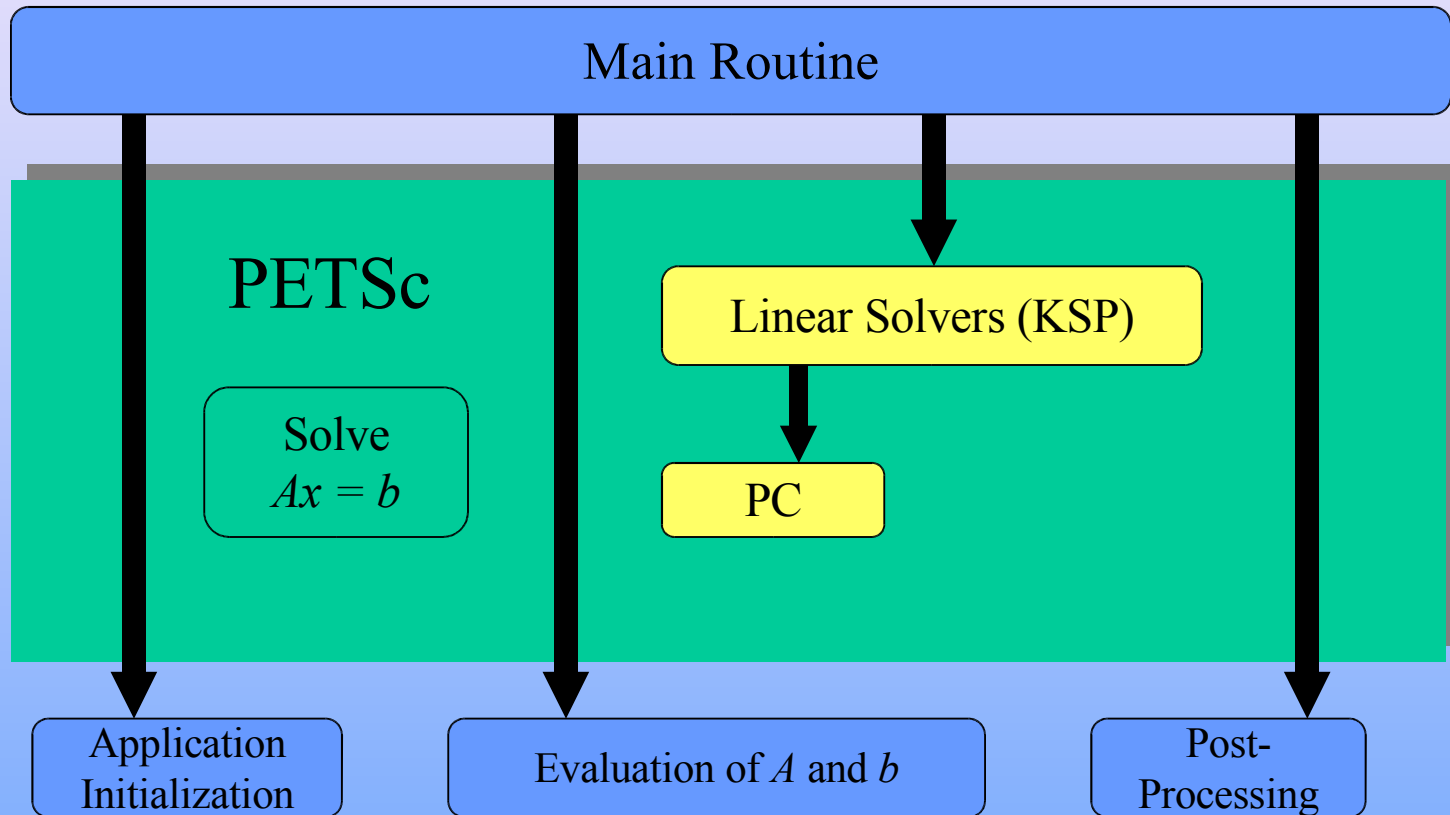data objects: matrices

Blocking: Performance Benefits

More issues discussed in full tutorials available via PETSc web site.

- 3D compressible Euler code
- Block size 5
- IBM Power2

data objects: matrices

Linear Solution

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)

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

beginner

solvers:
linear

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 via BlockSolve95
- ILU(k), LU (direct solve, sequential only)
- Arbitrary matrix
- etc.

beginner

solvers: linear

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,&its);
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

beginner

solvers:
linear

Basic Linear Solver Code (Fortran)

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

call  MatCreate( PETSC_COMM_WORLD,A,ierr )
call MatSetSizes(A,PETSC_DECIDE,PETSC_DECIDE,n,n,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,its,ierr)
call  KSPDestroy(ksp,ierr)
```

beginner

solvers:
linear

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

beginner

solvers:
linear

Setting Solver Options at Runtime

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

△ 1

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

⬠ 2

△ 1   ⬠ 2

| beginner | intermediate |

solvers:
linear

Linear Solvers: Monitoring Convergence

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

① 1

- -ksp_truemonitor — Prints true residual norm $\| b-Ax \|$
- -ksp_xtruemonitor — Plots true residual norm $\| b-Ax \|$

② 2

- User-defined monitors, using callbacks

③ 3

solvers:
linear

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....

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>

beginner

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

beginner

solvers:
linear

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>

And many more options...

△1 ⬠2

| beginner | intermediate |

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_xmonitor, -ksp_truemonitor, -ksp_xtruemonitor

△2

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...

△1 △2

beginner | 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

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

solvers:
linear

Viewing KSP Runtime Options

```
emacs@lava.mcs.anl.gov

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

solvers:
linear

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)

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/mat.h
- Some defaults provided for nonlinear solver usage

advanced

solvers:
linear

Nonlinear Solvers (SNES)

SNES: Scalable Nonlinear Equations Solvers

- Application code interface
- Choosing the solver
- Setting algorithmic options
- Viewing the solver
- Determining and monitoring convergence
- Matrix-free solvers
- User-defined customizations

solvers:
   nonlinear

Nonlinear Solvers

Goal: For problems arising from PDEs,
support the general solution of $F(u) = 0$

User provides:

- Code to evaluate $F(u)$
- Code to evaluate Jacobian of $F(u)$ (optional)
  - or use sparse finite difference approximation
  - or use automatic differentiation
    - AD support via collaboration with P. Hovland and B. Norris
    - Coming in next PETSc release via automated interface to ADIFOR and ADIC (see http://www.mcs.anl.gov/autodiff)

solvers:
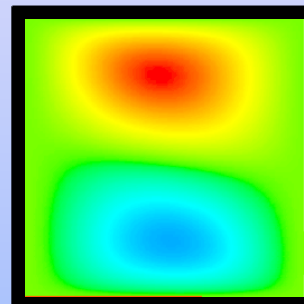nonlinear

Nonlinear Solvers (SNES)

- Newton-based methods, including
  - Line search strategies
  - Trust region approaches (using TAO)
  - Pseudo-transient continuation
  - Matrix-free variants
- Can customize all phases of solution process

solvers:
nonlinear

Sample Nonlinear Application:
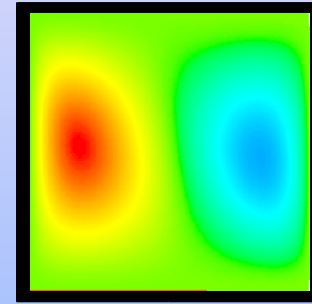## Driven Cavity Problem

- Velocity-vorticity formulation

- Flow driven by lid and/or bouyancy

- Logically regular grid, parallelized with DAs

- Finite difference discretization
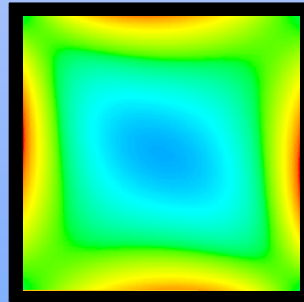
- source code:

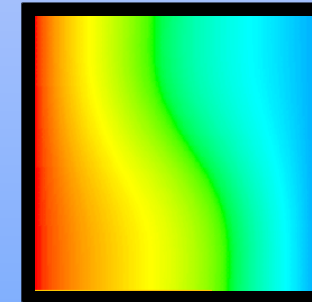petsc/src/snes/examples/tutorials/ex19.c

Application code author: D. E. Keyes

Solution Components

velocity: u

velocity: v

vorticity: z

temperature: T

solvers: nonlinear

Basic Nonlinear Solver Code (C/C++)

```
SNES     snes;                    /*  nonlinear solver context  */
Mat      J;                       /*  Jacobian matrix  */
Vec      x, F;                    /*  solution, residual vectors  */
int      n, its;                  /*  problem dimension, number of iterations  */
ApplicationCtx  usercontext;      /*  user-defined application context  */

…
MatCreate(PETSC_COMM_WORLD, &J);
MatSetSizes(J, PETSC_DECIDE,PETSC_DECIDE,n,n)
MatSetFromOptions(J);
VecCreate(PETSC_COMM_WORLD,&x);
VecSetSizes(x,PETSC_DECIDE,n);
VecSetFromOptions(x);
VecDuplicate(x,&F);

SNESCreate(PETSC_COMM_WORLD,&snes);
SNESSetFunction(snes,F,EvaluateFunction,usercontext);
SNESSetJacobian(snes,J,J,EvaluateJacobian,usercontext);
SNESSetFromOptions(snes);
SNESSolve(snes,x,&its);
SNESDestroy(snes);
```

solvers:
nonlinear

Solvers Based on Callbacks

- User provides routines to perform actions that the library requires. For example,
  - SNESSetFunction(SNES,...)
    - uservector - vector to store function values
    - userfunction - name of the user's function
    - usercontext - pointer to private data for the user's function

- Now, whenever the library needs to evaluate the user's nonlinear function, the solver may call the application code directly with its own local state.

- usercontext: serves as an application context object. Data are handled through such opaque objects; the library never sees irrelevant application data.

important concept

solvers:
nonlinear

Sample Application Context:
Driven Cavity Problem

```c
typedef struct {
    /* - - - - - - - - - - - - - basic application data - - - - - - - - - - - - - - - - */
    double        lid_velocity, prandtl;        /* problem parameters */
    double        grashof;                       /* problem parameters */
    int           mx, my;                        /* discretization parameters */
    int           mc;                   /* number of DoF per node */
    int           draw_contours;   /* flag - drawing contours */
    /* - - - - - - - - - - - - -     parallel data   - - - - - - - - - - - - - - - - - - - - */
    MPI_Comm  comm;                              /* communicator */
    DA            da;                   /* distributed array */
    Vec           localF, localX;   /* local ghosted vectors */
} AppCtx;
```

Sample Function Evaluation Code:
Driven Cavity Problem

```
UserComputeFunction(SNES snes, Vec X, Vec F, void *ptr)
{
    AppCtx   *user = (AppCtx *) ptr;           /* user-defined application context */
    int        istart, iend, jstart, jend;      /* local starting and ending grid points */
    Scalar    *f;                               /* local vector data */

    ….
    /* (Code to communicate nonlocal ghost point data not shown) */
    VecGetArray( F, &f );
    /* (Code to compute local function components; insert into f[ ] shown on next slide) */
    VecRestoreArray( F, &f );

    ….
return 0;
}
```

solvers:
nonlinear

Sample Local Computational Loops:
Driven Cavity Problem

```
….
for ( j = jstart;  j<jend;  j++ )  {
    row = (j - gys) * gxm + istart - gxs - 1;
    for ( i = istart; i<iend; i++ )  {
        row++;    u = x[row].u;
        uxx = (two * u - x[row-1].u - x [ row+1 ].u ) * hydhx;
        uyy = (two * u - x[row-gxm].u - x [row+gxm].u * hxdhy;
        f [row].u = uxx + uyy –
            p5 * (x [row+gxm].omega- x [row-gxm].omega) * hx;
        …..
} }
    ….
```

- The PDE's 4 components (U,V,Omega,Temp) are interleaved in the unknown vector.
- #define statements provide easy access to each component.

solvers:
nonlinear

Finite Difference Jacobian Computation

- Compute and explicitly store Jacobian via 1st-order FD
  - Dense: -snes_fd, SNESDefaultComputeJacobian()
  - Sparse via colorings: MatFDColoringCreate(), SNESDefaultComputeJacobianColor()
- Matrix-free Newton-Krylov via 1st-order FD, no preconditioning unless specifically set by user
  - -snes_mf
- Matrix-free Newton-Krylov via 1st-order FD, user-defined preconditioning matrix
  - -snes_mf_operator

solvers:
nonlinear

Uniform access to all linear and nonlinear solvers

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

1

- -snes_line_search <line search method>
- -sles_ls <parameters>
- -snes_convergence <tolerance>
- etc...

2

solvers:
nonlinear

Customization via Callbacks:
Setting a user-defined line search routine

SNESSetLineSearch(SNES snes,int(*ls)(…),void *lsctx)

Available line search routines ls( ) include:

- SNESCubicLineSearch( ) - cubic line search
- SNESQuadraticLineSearch( ) - quadratic line search
- SNESNoLineSearch( ) - full Newton step
- SNESNoLineSearchNoNorms( ) - full Newton step but calculates no norms (faster in parallel, useful when using a fixed number of Newton iterations instead of usual convergence testing)
- YourOwnFavoriteLineSearchRoutine( )

solvers:
nonlinear

SNES: Review of Basic Usage

- SNESCreate( )   - Create SNES context
- SNESSetFunction( )   - Set function eval. routine
- SNESSetJacobian( )   - Set Jacobian eval. routine
- SNESSetFromOptions( )   - Set runtime solver options
                                for [SNES,SLES, KSP,PC]
- SNESSolve( )   - Run nonlinear solver
- SNESView( )   - View solver options
                         actually used at runtime
                         (alternative: -snes_view)
- SNESDestroy( )   - Destroy solver

solvers:
nonlinear

SNES: Review of Selected Options

Functionality	Procedural Interface	Runtime Option
Set nonlinear solver	SNESSetType( )	-snes_type [ls,tr,umls,umtr,…]
Set monitoring routine	SNESSetMonitor( )	-snes_monitor –snes_xmonitor, …

Functionality	Procedural Interface	Runtime Option
Set convergence tolerances	SNESSetTolerances( )	-snes_rtol <rt> -snes_atol <at> -snes _max_its <its>
Set line search routine	SNESSetLineSearch( )	-snes_eq_ls [cubic,quadratic,…]
View solver options	SNESView( )	-snes_view
Set linear solver options	SNESGetSLES( ) SLESGetKSP( ) SLESGetPC( )	-ksp_type <ksptype> -ksp_rtol <krt> -pc_type <pctype> …

And many more options...

solvers:
nonlinear

Not so
Advanced PETSc

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

Integration

Debugging

Support for parallel debugging

- -start_in_debugger [gdb,dbx,noxterm]

- -on_error_attach_debugger [gdb,dbx,noxterm]

- -on_error_abort

- -debugger_nodes 0,1

- -display machinename:0.0

When debugging, it is often useful to place a breakpoint in the function PetscError( ).

debugging and errors

Sample Error Traceback

Breakdown in ILU factorization due to a zero pivot


```
xterm

Buffers Files Tools Edit Search Mule Help
[dreamcast] mpirun -np 1 ex1
-----------------------------------------------------------------
PETSc Version 2.1.0, Released April 11, 2001
        The PETSc Team     petsc-maint@mcs.anl.gov
 http://www.mcs.anl.gov/petsc/

See docs/copyright.html for copyright information.
See docs/changes.html for recent updates.
See docs/troubleshooting.html for hints about trouble shooting.
See docs/manualpages/index.html for manual pages.
-----------------------------------------------------------------
ex1 on a linux named dreamcast.mcs.anl.gov by balay Thu Oct  4 15:25:11 2001
Libraries linked from /home/balay/software/petsc-2.1.0/lib/libg/linux
-----------------------------------------------------------------
[0]PETSC ERROR: MatLUFactorNumeric_SeqAIJ() line 508 in src/mat/impls/aij/seq/aijfact.c
[0]PETSC ERROR:    Detected zero pivot in LU factorization!
[0]PETSC ERROR:    Zero pivot row 0!
[0]PETSC ERROR: MatLUFactorNumeric() line 1575 in src/mat/interface/matrix.c
[0]PETSC ERROR: PCSetUp_ILU() line 646 in src/sles/pc/impls/ilu/ilu.c
[0]PETSC ERROR: PCSetUp() line 783 in src/sles/pc/interface/precon.c
[0]PETSC ERROR: SLESSetUp() line 382 in src/sles/interface/sles.c
[0]PETSC ERROR: SLESSolve() line 483 in src/sles/interface/sles.c
[0]PETSC ERROR: main() line 195 in test/ex1.c
[0] MPI Abort by user Aborting program !
[0] Aborting program!
p0_5469:  p4_error: : 71
--1-:---F1  logs              (Text)--L3-- 2%--------------------------------
```

debugging and errors

Sample Memory Corruption Error

```
xterm

Buffers Files Tools Edit Search Mule Help
[dreamcast] mpirun -np 1 ex2 -trmalloc_off
[dreamcast] mpirun -np 1 ex2 -trmalloc
------------------------------------------------------------

PETSc Version 2.1.0, Released April 11, 2001
        The PETSc Team    petsc-maint@mcs.anl.gov
 http://www.mcs.anl.gov/petsc/

See docs/copyright.html for copyright information.
See docs/changes.html for recent updates.
See docs/troubleshooting.html for hints about trouble shooting.
See docs/manualpages/index.html for manual pages.
------------------------------------------------------------
ex2 on a linux named dreamcast.mcs.anl.gov by balay Thu Oct  4 15:35:29 2001
Libraries linked from /home/balay/software/petsc-2.1.0/lib/libg/linux
------------------------------------------------------------
PetscTrFreeDefault called from main() line 51 in test/ex2.c
Block [id=0(14)] at address 0x81152d8 is corrupted (probably write past end)
Block allocated in main() line 49 in test/ex2.c
[0]PETSC ERROR: PetscTrFreeDefault() line 363 in src/sys/src/memory/mtr.c
[0]PETSC ERROR:   Memory corruption!
[0]PETSC ERROR:   Corrupted memory!
[0]PETSC ERROR: main() line 51 in test/ex2.c
[0] MPI Abort by user Aborting program !
[0] Aborting program!
p0_5691:  p4_error: : 78
--1-:---F1  logs              (Text)--L32--27%------------------------------------
```

debugging and errors

Sample Out-of-Memory Error

```
xterm                                                              _ □ ✕
Buffers Files Tools Edit Search Mule Help
[dreamcast] mpirun -np 1 ex3
----------------------------------------------------------------
PETSc Version 2.1.0, Released April 11, 2001
        The PETSc Team     petsc-maint@mcs.anl.gov
 http://www.mcs.anl.gov/petsc/

See docs/copyright.html for copyright information.
See docs/changes.html for recent updates.
See docs/troubleshooting.html for hints about trouble shooting.
See docs/manualpages/index.html for manual pages.
----------------------------------------------------------------
ex3 on a linux named dreamcast.mcs.anl.gov by balay Thu Oct  4 15:51:46 2001
Libraries linked from /home/balay/software/petsc-2.1.0/lib/libg/linux
----------------------------------------------------------------
[0]PETSC ERROR: PetscMallocAlign() line 59 in src/sys/src/memory/mal.c
[0]PETSC ERROR:    Out of memory. This could be due to allocating
[0]PETSC ERROR:    too large an object or bleeding by not properly
[0]PETSC ERROR:    destroying unneeded objects.
[0]PETSC ERROR:    Memory allocated -2044966576 Memory used by process 0
[0]PETSC ERROR:    Try running with -trdump or -trmalloc_log for info.
[0]PETSC ERROR:    Memory requested 500000296!
[0]PETSC ERROR: main() line 51 in test/ex3.c
[0] MPI Abort by user Aborting program !
[0] Aborting program!
p0_6291:  p4_error: : 55
--1-:---F1  logs                (Text)--L60--49%-----------------------
```

debugging and errors

Sample Floating Point Error


```
xterm

Buffers Files Tools Edit Search Mule Help

[maple] mpirun -np 1 ex4 -fp_trap
----------------------------------------------------------------
ex4 on a solaris named maple.mcs.anl.gov by balay Thu Oct  4 16:08:19 2001
Libraries linked from /homes/balay/spetsc/lib/libg/solaris

--------------- Stack Frames ---------------
Note: The EXACT line numbers in the stack are not available,
      INSTEAD the line number of the start of the function
      is given.
[0] CreateError line 12 tests/ex4.c
----------------------------------------------------------------
[0]PETSC ERROR: unknownfunction() line 0 in Unknown directoryUnknown file
[0]PETSC ERROR:    Signal received!
[0]PETSC ERROR:    Caught signal FPE:
PETSC ERROR: Floating Point Exception,probably divide by zero
PETSC ERROR: Try option -start_in_debugger or -on_error_attach_debugger to
PETSC ERROR: determine where problem occurs
PETSC ERROR: likely location of problem given above in stack
!
[0] MPI Abort by user Aborting program !
[0] Aborting program!
p0_20924:  p4_error: : 59


--1-:---F1   logs               (Text)--L88--Bot-----------------------------
```

debugging and errors

Profiling and Performance Tuning

Profiling:

- Integrated profiling using -log_summary

- User-defined events

- Profiling by stages of an application

Performance Tuning:

- Matrix optimizations

- Application optimizations

- Algorithmic tuning

profiling and
performance tuning

Profiling

- Integrated monitoring of
  - time
  - floating-point performance
  - memory usage
  - communication
- Active if PETSc was compiled with -DPETSC_LOG (default)
  - Can also profile application code segments
- Print summary data with option: -log_summary
- Print redundant information from PETSc routines: -log_info
- Print the trace of the functions called: -log_trace

profiling and
performance tuning

Sample -log_summary

```
-----------------------------------------------------------------------------------------------------------------
Event                Count       Time (sec)      Flops/sec                              --- Global ---  --- Stage ---   Total
                   Max Ratio  Max     Ratio   Max   Ratio  Mess   Avg len  Reduct      %T %F %M %L %R   %T %F %M %L %R   Mflop/s
-----------------------------------------------------------------------------------------------------------------

--- Event Stage 0: Main Stage

PetscBarrier          2 1.0 1.1733e-05 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00   0  0  0  0  0   0  0  0  0  0      0

--- Event Stage 1: SetUp

VecSet                2 1.0 9.3448e-04 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00   0  0  0  0  0   0  0  0  0  0      0
MatMultTranspose      1 1.0 1.8022e-03 1.0 1.85e+08 1.0 0.0e+00 0.0e+00 0.0e+00   0  0  0  0  0   0 57  0  0  0    185
MatAssemblyBegin      3 1.0 1.0057e-05 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00   0  0  0  0  0   0  0  0  0  0      0
MatAssemblyEnd        3 1.0 2.0356e-02 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 0.0e+00   0  0  0  0  0   5  0  0  0  0      0
MatFDColorCreate      2 1.0 1.5341e-01 1.0 0.00e+00 0.0 0.0e+00 0.0e+00 4.6e+01   1  0  0  0 16  36  0  0  0 74      0

--- Event Stage 2: Solve

VecDot                2 1.0 3.2985e-03 1.0 9.56e+07 1.0 0.0e+00 0.0e+00 2.0e+00   0  0  0  0  1   0  0  0  0  2     96
VecMDot              45 1.0 9.3093e-02 1.0 1.59e+08 1.0 0.0e+00 0.0e+00 1.5e+01   0  0  0  0  5   1  1  0  0 19    159
VecNorm             112 1.0 2.0851e-01 1.0 8.47e+07 1.0 0.0e+00 0.0e+00 5.2e+01   1  1  0  0 18   2  1  0  0 64     85
```

```
MatMultTranspose    1 1.0 1.8022e-03 1.0 1.85e+08 ...
VecNorm           112 1.0 2.0851e-01 1.0 8.47e+07 ... 5.2e+01 …
```

More –log_summary

```
Memory usage is given in bytes:

Object Type            Creations    Destructions    Memory  Descendants' Mem.

--- Event Stage 0: Main Stage


--- Event Stage 1: SetUp

   Distributed array      4               0           0    2.37475e+06
          Index Set     104              24     2376480    0
                Map      40              10        2000    0
                Vec      36              10     2846384    0
        Vec Scatter      12               0           0    0
IS Local to global mapping      8            0           0    0
             Matrix       8               0           0    0
  Matrix FD Coloring      4               0           0    0
               SNES      4               0           0    0
     Krylov Solver      10               0           0    0
     Preconditioner     10               0           0    0

--- Event Stage 2: Solve

   Distributed array      0               4      822496    3.16488e+06
          Index Set      20             100     3578544    0
                Map      26              56       11200    0
                Vec     160             186    92490656    2864
        Vec Scatter       0              12     2374784    0
```

Still more –log_summary

```
================================================================================
Average time to get PetscTime(): 1.13389e-08
Compiled without FORTRAN kernels
Compiled with double precision matrices (default)
sizeof(short) 2 sizeof(int) 4 sizeof(long) 4 sizeof(void*) 4
Libraries compiled on Fri May 28 01:39:58 PDT 2004 on MBuschel
Machine characteristics: CYGWIN_NT-5.1 MBuschel 1.5.9(0.112/4/2) 2004-03-18 23:05
Using PETSc directory: /home/Kris/petsc/petsc-dev
Using PETSc arch: cygwin
-----------------------------------------
Using C compiler: gcc -Wall -O -fomit-frame-pointer -Wno-strict-aliasing -I/home/K
c-dev/bmake/cygwin -I/home/Kris/petsc/petsc-dev/include   -I/software/MPI/mpich-nt

EXTERN_CXX  -D__SDIR__='. '
C Compiler version:
gcc (GCC) 3.3.1 (cygming special)\nCopyright (C) 2003 Free Software Foundation,
```

Adding a new Stage

```
int stageNum;
PetscLogStageRegister(&stageNum,"name");



PetscLogStagePush(stageNum);
[code to monitor]
PetscLogStagePop();
```

profiling and
performance tuning

Adding a new Event

```
static int USER_EVENT;
PetscLogEventRegister(&USER_EVENT,"name",CLASS_COOKIE);


PetscLogEventBegin(USER_EVENT,0,0,0,0);
[code to monitor]
PetscLogFlops(user_evnet_flops);
PetscLogEventEnd(USER_EVENT,0,0,0,0);
```

profiling and
performance tuning

Adding a new Class

- Cookie identifies a class uniquely

```
static int CLASS_COOKIE;
PetscLogClassRegister(&CLASS_COOKIE,"name");
```

- This initialization must happen before any objects of this type are created

profiling and
performance tuning

Performance Requires Managing Memory

- Real systems have many levels of memory
  - Programming models try to hide memory hierarchy
    - Except C—`register`
- Simplest model: Two levels of memory
  - Divide at largest (relative) latency gap
  - Processes have their own memory
    - Managing a processes memory is known (if unsolved) problem
  - Exactly matches the distributed memory model

profiling and
performance tuning

Sparse Matrix-Vector Product

- Common operation for optimal (in floating-point operations) solution of linear systems
- Sample code:

```
for row=0,n-1
    m   = i[row+1] - i[row];
    sum = 0;
    for k=0,m-1
        sum += *a++ * x[*j++];
    y[row] = sum;
```

- Data structures are a[nnz], j[nnz], i[n], x[n], y[n]

profiling and
performance tuning

Simple Performance Analysis

- Memory motion:
  - nnz (sizeof(double) + sizeof(int)) + n (2*sizeof(double) + sizeof(int))
  - Perfect cache (never load same data twice)
- Computation
  - nnz multiply-add (MA)
- Roughly 12 bytes per MA
- Typical WS node can move ½-4 bytes/MA
  - *Maximum* performance is 4-33% of peak

profiling and performance tuning

More Performance Analysis

- Instruction Counts:
  - nnz (2*load-double + load-int + mult-add) +
    n (load-int + store-double)
- Roughly 4 instructions per MA
- Maximum performance is 25% of peak (33% if MA overlaps one load/store)
- Changing matrix data structure (e.g., exploit small block structure) allows reuse of data in register, eliminating some loads (x and j)
- Implementation improvements (tricks) cannot improve on these limits

profiling and
performance tuning

Alternative Building Blocks

- Performance of sparse matrix - multi-vector multiply:

Format	Number of Vectors	Mflops	
		Ideal	Achieved
AIJ	1	49	45
AIJ	4	182	120
BAIJ	1	64	55
BAIJ	4	236	175

- Results from 250 MHz R10000 (500 MF/sec peak)

- BAIJ is a block AIJ with blocksize of 4

- Multiple right-hand sides can be solved in nearly the same time as a single RHS

profiling and performance tuning

Matrix Memory Pre-allocation

- PETSc sparse matrices are dynamic data structures. Can add additional nonzeros freely

- Dynamically adding many nonzeros
  - requires additional memory allocations
  - requires copies
  - can kill performance

- Memory pre-allocation provides the freedom of dynamic data structures plus good performance

profiling and
performance tuning

Indicating Expected Nonzeros
Sequential Sparse Matrices

MatCreateSeqAIJ(...., int *nnz,Mat *A)

- nnz[0] - expected number of nonzeros in row 0

- nnz[1] - expected number of nonzeros in row 1

row 0
row 1
row 2
row 3

sample nonzero pattern
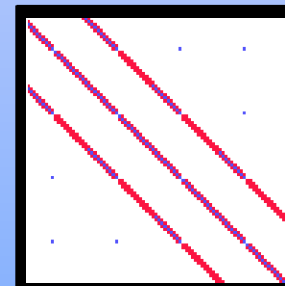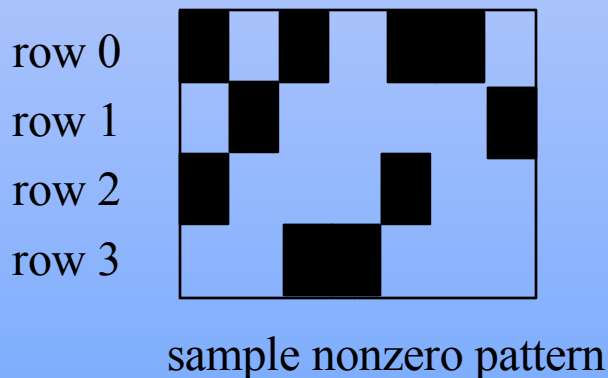
another sample

nonzero pattern

profiling and
performance tuning

Symbolic Computation of Matrix Nonzero Structure

- Create matrix with MatCreate()
- Set type with MatSetType()
- Form the nonzero structure of the matrix
  - loop over the grid for finite differences
  - loop over the elements for finite elements
  - etc.
- Preallocate matrix
  - MatSeqAIJSetPreallocation()
  - MatMPIAIJSetPreallocation()

profiling and
performance tuning

Parallel Sparse Matrices

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

- Each submatrix consists of **diagonal** and **off-diagonal** parts.

proc 0
proc 1
proc 2
proc 3
proc 4

■ diagonal portions
□ off-diagonal portions

} proc 3: locally owned rows

profiling and
performance tuning
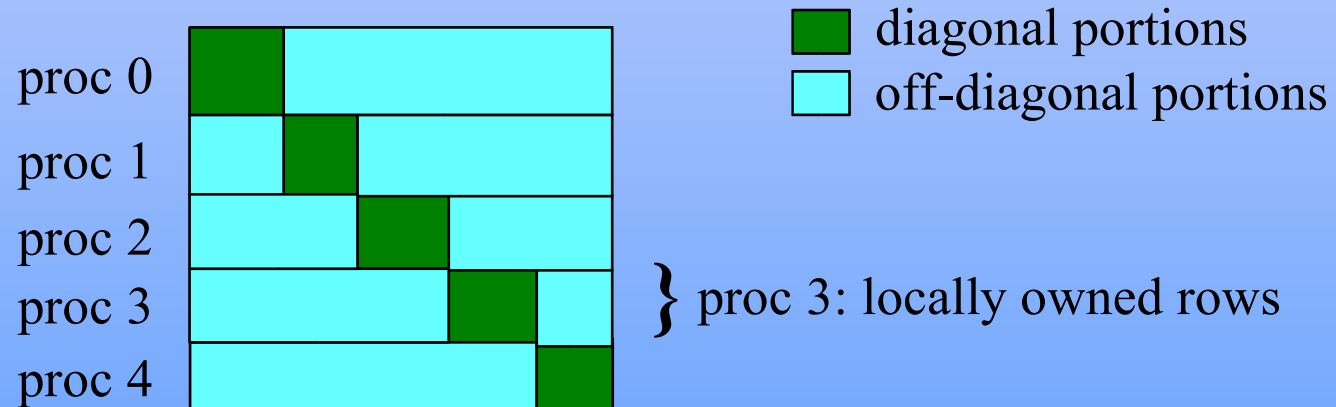
Indicating Expected Nonzeros
Parallel Sparse Matrices

```
MatMPIAIJSetPreallocation(Mat A,
                          int d_nz, int *d_nnz,
                          int o_nz, int *o_nnz)
```

- `d_nnz[]` - expected number of nonzeros per row in diagonal portion of local submatrix

- `o_nnz[]` - expected number of nonzeros per row in off-diagonal portion of local submatrix

profiling and
performance tuning

Verifying Predictions

- Use runtime option: -log_info

- Output:

  [proc #] Matrix size: %d X %d; storage space: %d unneeded, %d used

  [proc #] Number of mallocs during MatSetValues( ) is %d

```
[merlin] mpirun ex2 -log_info
[0]MatAssemblyEnd_SeqAIJ:Matrix size: 56 X 56; storage space:
[0]    310 unneeded, 250 used
[0]MatAssemblyEnd_SeqAIJ:Number of mallocs during MatSetValues() is 0
[0]MatAssemblyEnd_SeqAIJ:Most nonzeros in any row is 5
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routines
[0]Mat_AIJ_CheckInode: Found 56 nodes out of 56 rows. Not using Inode routines
Norm of error 0.000156044 iterations 6
[0]PetscFinalize:PETSc successfully ended!
```

profiling and
performance tuning

Extending PETSc

Linking to PETSc

- Application program or framework
- Nothing but the libraries
  - Custom link by user
- Using the PETSc build variables
  - Include bmake/common/variables
- Using the PETSc build rules
  - Include bmake/common/base
  - Also makes available 3rd party packages

Extending PETSc

Customizing the Framework

- Adding additional logging
  - Pushing new stages
  - Registering new events and logging classes
- Adding 3rd party PETSc libraries
  - Enlarging the dynamic link path

Adding an Implementation

- See `src/ksp/pc/impls/jacobi/jacobi.c`
- Implement the interface methods
  - For Jacobi, PCSetUp(), PCApply(),…
- Define a constructor
  - Allocate and initialize the class structure
  - Fill in the function table
  - Must have C linkage
- Register the constructor
  - See `src/ksp/ksp/interface/dlregis.c`
  - Maps a string (class name) to the constructor
  - Usually uses PetscFListAdd()

Extending PETSc

Adding a Wrapper

- See `src/ts/impls/implicit/pvode/petscpvode.c`

- Just like an Implementation

  - Methods dispatch to 3rd party software

- Need to alter local makefile

  - Add a `requirespackage` line

  - Add include variable to `CPPFLAGS`

- Also need usual configure build additions

Adding a Subtype

- See `src/mat/impls/aij/seq/umfpack/umfpack.c`

- Have to virtualize methods by hand

- Define a constructor
  - Change type name first to correct name
  - Call MatSetType() for base type
  - Replace (and save) overidden methods
  - Construct any specific data

- Must also define a conversion to the base type
  - Only called in destructor right now

Adding a Type I

- See `src/ksp/ksp/kspimpl.h`

- Define a methods structure (interface)
  - A list of function pointers

- Define a type structure
  - First member is `PETSCHEADER(struct _Ops)`
  - Possibly other data members common to the type
  - A `void *data` for implementation structures

Extending PETSc

Adding a Type II

- See `src/ksp/ksp/interface/dlregis.c`

- Define a package initializer (`PetscDLLibraryRegister`)
  - Called when the DLL is loaded
    - Also called from generic create if linking statically
  - Registers classes and events (see below)
  - Registers any default implementation constructors
  - Setup any info or summary exclusions

Extending PETSc

Adding a Type III

- See `src/ksp/ksp/interface/itcreate.c`
- Define a generic create
  - Call package initializer if linking statically
  - Call `PetscHeaderCreate()`
  - Initialize any default data members
- Define a `setType()` method
  - Call the destructor of any current implementation
  - Call the constructor of the given implementation
  - Set the type name

Adding a Type IV

- Things swept under the rug
  - Want a `setFromOptions()` which allows selection of implementations at runtime
  - Have to manage the database of registered constructors
  - View and destroy functions handled a little funny due to historical reasons

Extending PETSc

Parallel Data Layout and Ghost Values: Usage Concepts

Managing field data layout and required ghost values is the key to high performance of most PDE-based parallel programs.

Mesh Types

- Structured
  - DA objects
- Unstructured
  - VecScatter objects

Usage Concepts

- Geometric data
- Data structure creation
- Ghost point updates
- Local numerical computation

important concepts

data layout

Ghost Values

Local node ●   Ghost node ○
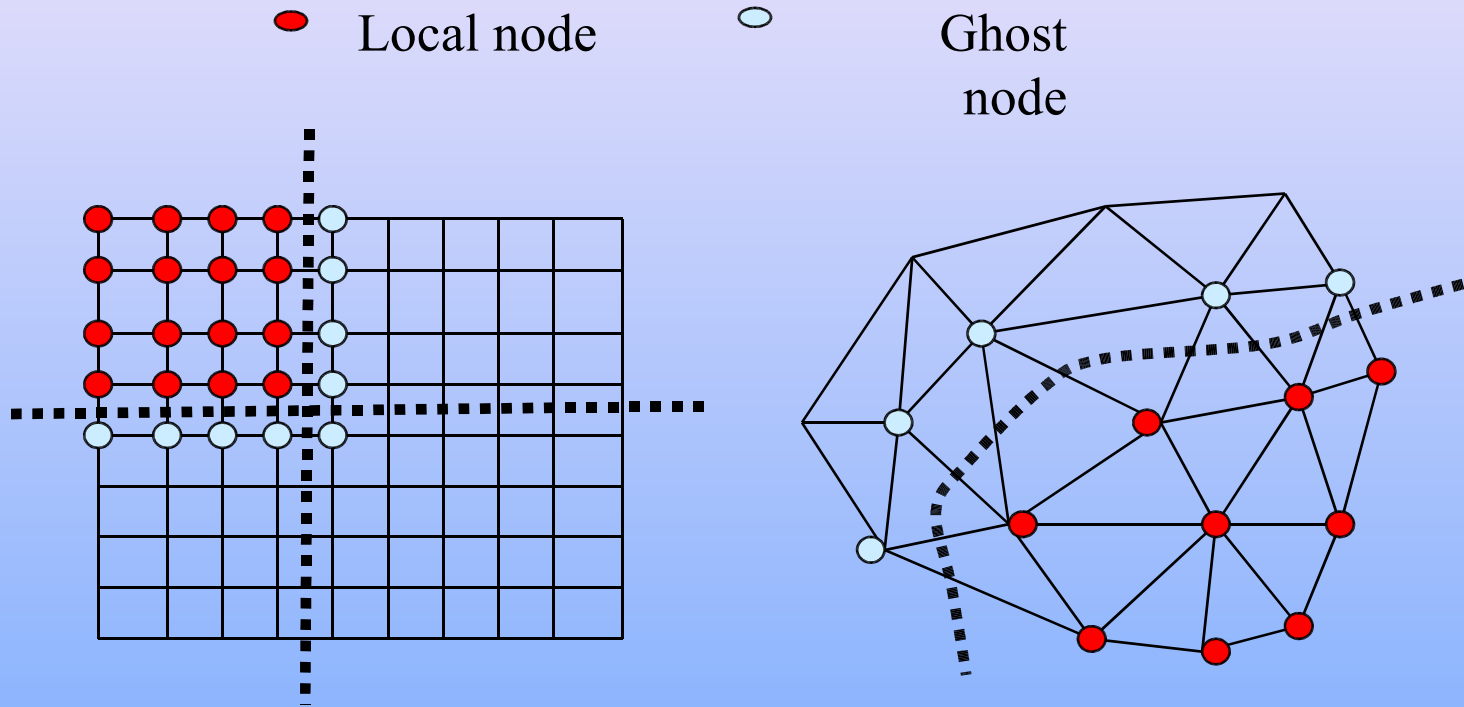
Ghost values: To evaluate a local function $f(x)$, each process requires its local portion of the vector x as well as its **ghost values** – or bordering portions of x that are owned by neighboring processes.

data layout

Communication and Physical Discretization

Communication				Local Numerical Computation
Geometric Data	Data Structure Creation	Ghost Point Data Structures	Ghost Point Updates	

stencil [implicit]   DACreate( )   DA AO   DAGlobalToLocal( )   Loops over I,J,K indices

structured meshes △1

elements edges vertices   VecScatterCreate( )   VecScatter AO   VecScatter( )   Loops over entities

unstructured meshes ⬠2
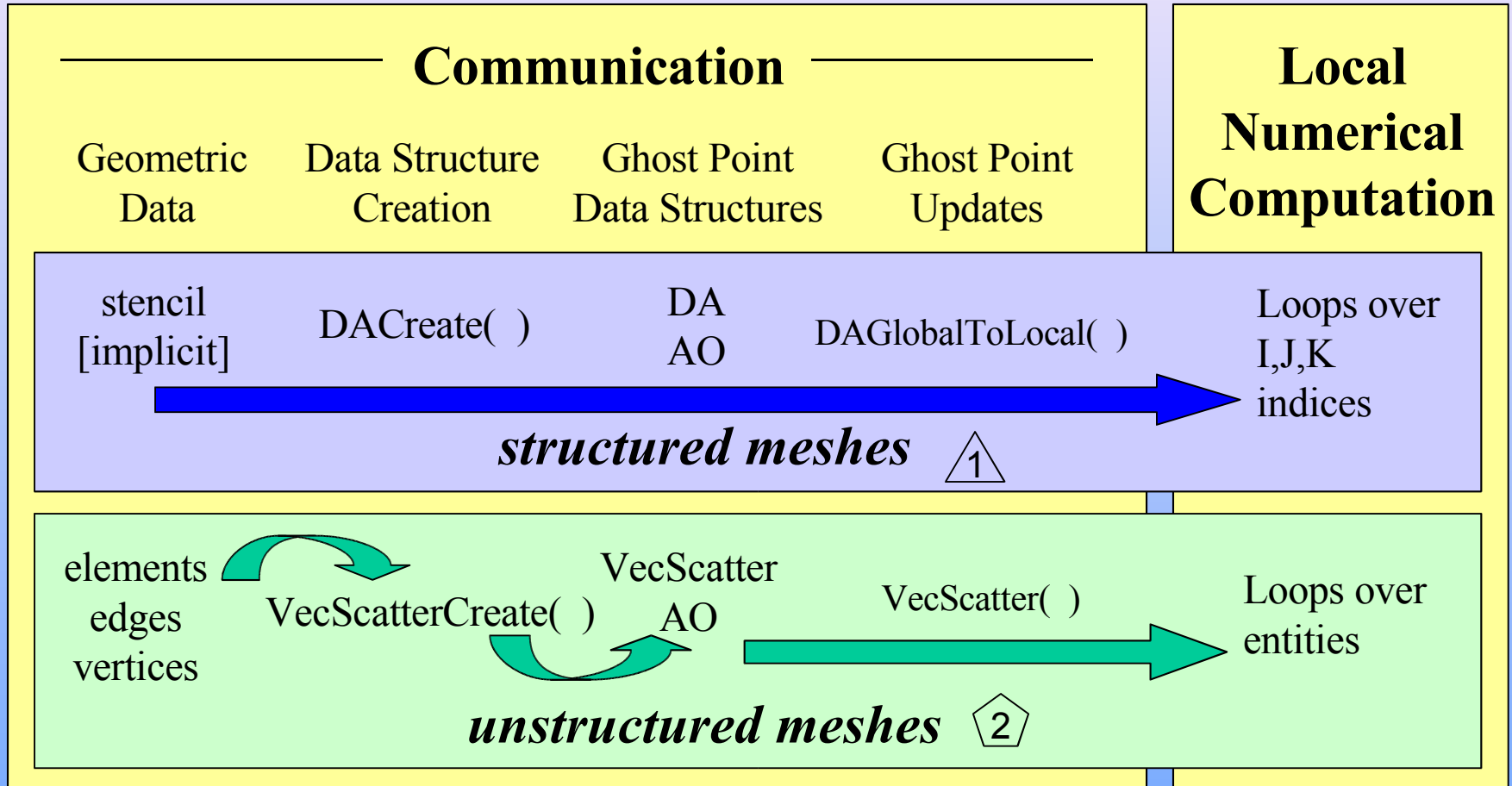
data layout

DA: Parallel Data Layout and Ghost Values for Structured Meshes

- Local and global indices

- Local and global vectors

- DA creation

- Ghost point updates

- Viewing

data layout:
distributed arrays

Communication and Physical Discretization: Structured Meshes

Communication				Local Numerical Computation
Geometric Data	Data Structure Creation	Ghost Point Data Structures	Ghost Point Updates	
stencil [implicit]	DACreate( )	DA AO	DAGlobalToLocal( )	Loops over I,J,K indices

structured meshes
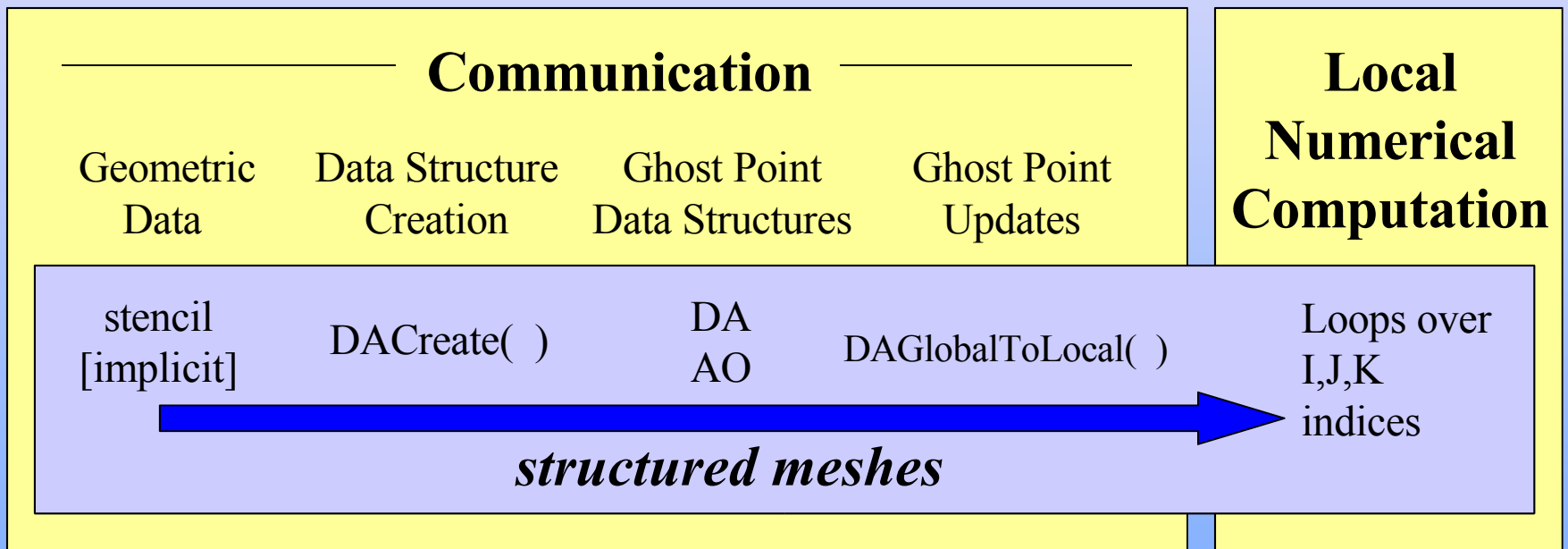
data layout: distributed arrays

Global and Local Representations

Local node
Ghost node

5   9

0   1   2   3   4
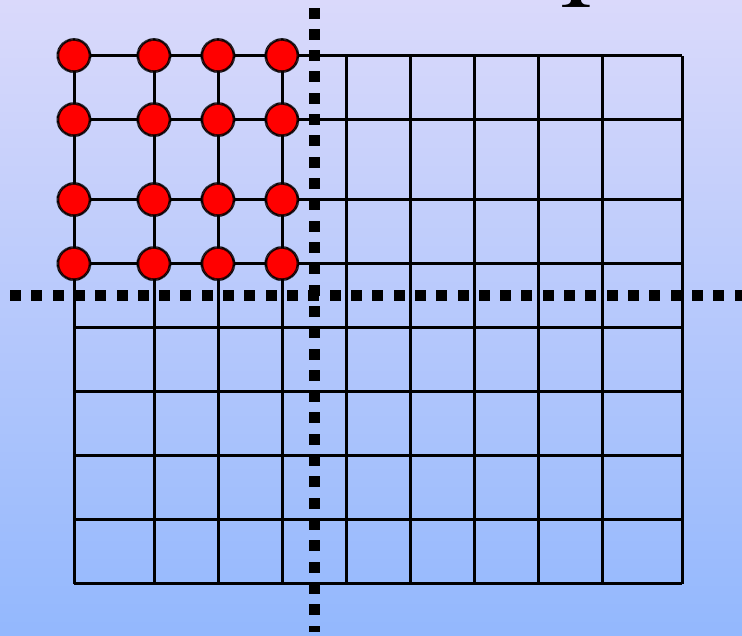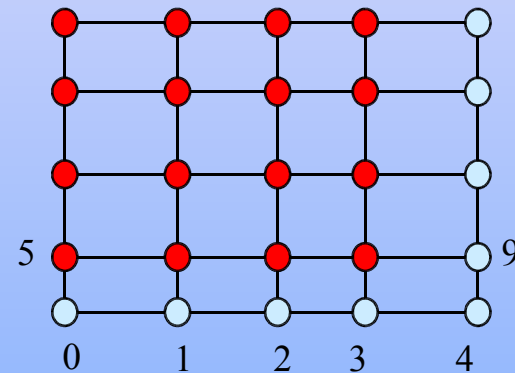
Global: each process stores a unique local set of vertices (and each vertex is owned by exactly one process)

Local: each process stores a unique local set of vertices *as well as* ghost nodes from neighboring processes

data layout: distributed arrays

Global and Local Representations (cont.)
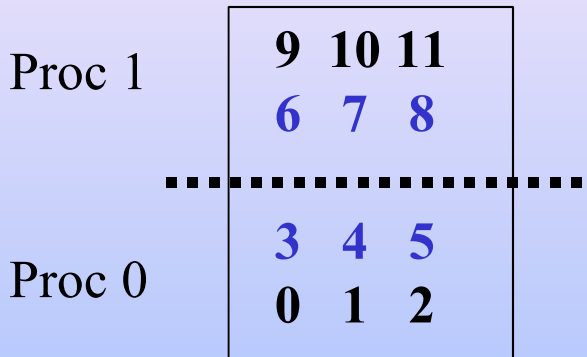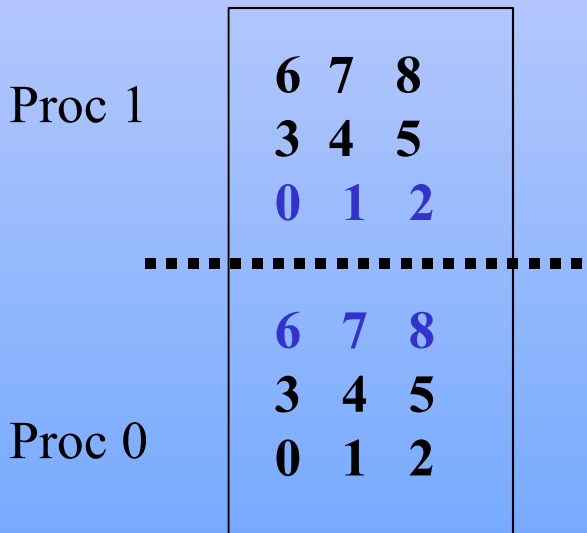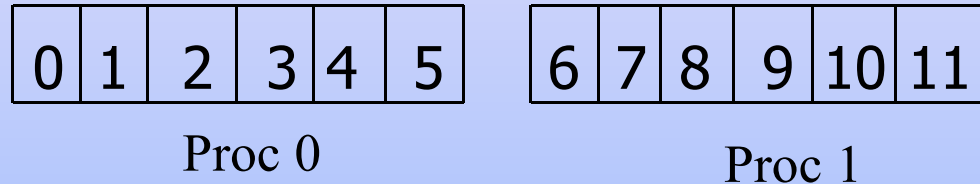
Logically Regular Meshes

- DA - Distributed Array: object containing information about vector layout across the processes and communication of ghost values

- Form a DA
  - DACreate1d(....,DA *)
  - DACreate2d(....,DA *)
  - DACreate3d(....,DA *)

- Create the corresponding PETSc vectors
  - DACreateGlobalVector(DA, Vec *) or
  - DACreateLocalVector(DA, Vec *)

- Update ghostpoints (scatter global vector into local parts, including ghost points)
  - DAGlobalToLocalBegin(DA, …)
  - DAGlobalToLocalEnd(DA,…)

data layout:
distributed arrays

Distributed Arrays

Data layout and ghost values
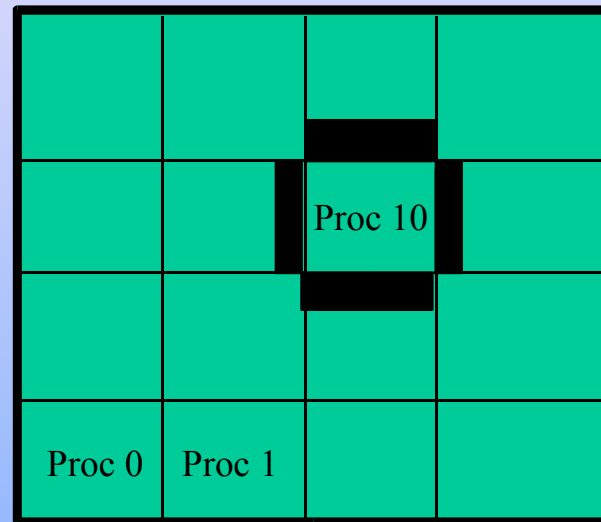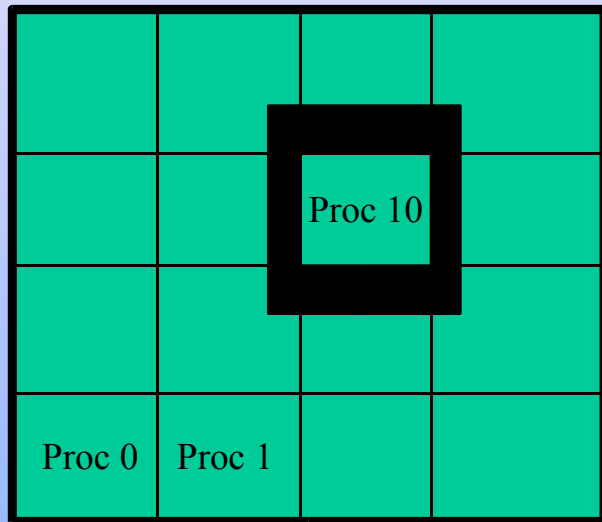
Box-type stencil
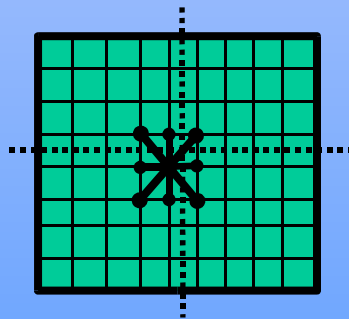
Star-type stencil
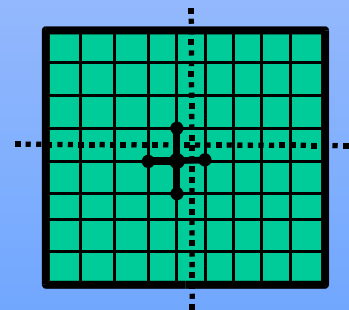
data layout: distributed arrays

Vectors and DAs

- The DA object contains information about the data layout and ghost values, but **not** the actual field data, which is contained in PETSc vectors

- Global vector: parallel
  - each process stores a unique local portion
  - DACreateGlobalVector(DA da,Vec *gvec);

- Local work vector: sequential
  - each process stores its local portion plus ghost values
  - DACreateLocalVector(DA da,Vec *lvec);
  - uses "natural" local numbering of indices (0,1,…*nlocal*-1)

data layout:
distributed arrays

DACreate1d(…,*DA)

- DACreate1d(MPI_Comm comm,DAPeriodicType wrap,
  int M,int dof,int s,int *lc,DA *inra)
  - MPI_Comm — processes containing array
  - DA_[NONPERIODIC,XPERIODIC]
  - number of grid points in x-direction
  - degrees of freedom per node
  - stencil width
  - Number of nodes for each domain
    - Use PETSC_NULL for the default

data layout:
distributed arrays

DACreate2d(...,*DA)

- DACreate2d(MPI_Comm comm,DAPeriodicType wrap,
  DAStencilType stencil_type, int M,int N,
  int m,int n,int dof,int s,int *lx,int *ly,DA *inra)
  - DA_[NON,X,Y,XY]PERIODIC
  - DA_STENCIL_[STAR,BOX]
  - number of grid points in x- and y-directions
  - processes in x- and y-directions
  - degrees of freedom per node
  - stencil width
  - Number of nodes for each domain
    - Use PETSC_NULL for the default

data layout:
distributed arrays

Updating the Local Representation

Two-step process enables overlapping computation and communication

- DAGlobalToLocalBegin(DA, global_vec, insert,local_vec)
  - global_vec provides data
  - Insert is either INSERT_VALUES or ADD_VALUES
    - specifies how to update values in the local vector
  - local_vec is a pre-existing local vector
- DAGlobalToLocal End(DA,…)
  - Takes same arguments

data layout:
distributed arrays

Ghost Point Scatters:
Burger's Equation Example

```
call DAGlobalToLocalBegin(da,u_global,INSERT_VALUES,ulocal,ierr)
call DAGlobalToLocalEnd(da,u_global,INSERT_VALUES,ulocal,ierr)

call VecGetArray( ulocal, uv, ui, ierr )
#define u(i) uv(ui+i)
C  Do local computations (here u and f are local vectors)
   do 10, i=1,localsize
      f(i) = (.5/h)*u(i)*(u(i+1) - u(i-1)) + (e/(h*h))*(u(i+1) - 2.0*u(i) + u(i-1))
10  continue
   call VecRestoreArray( ulocal, uv, ui, ierr )
   call DALocalToGlobal(da,f,INSERT_VALUES,f_global,ierr)
```
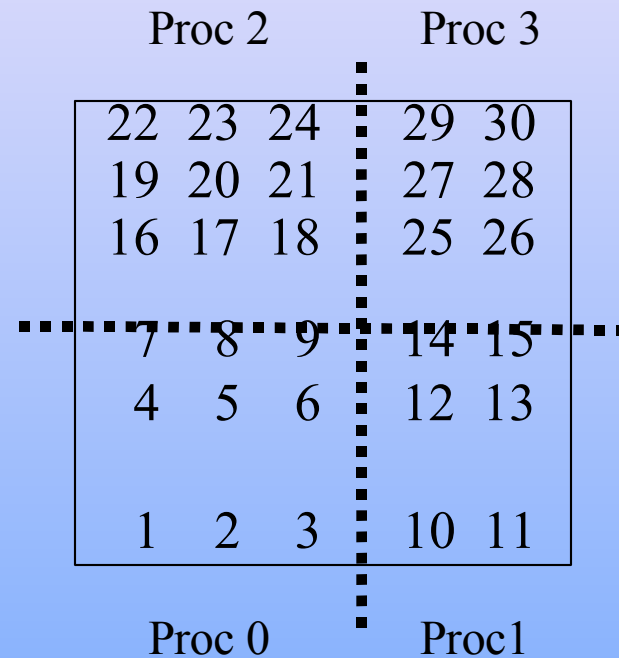
data layout:
distributed arrays

Global Numbering used by DAs

Proc 2   Proc 3

26	27	28	29	30
21	22	23	24	25
16	17	18	19	20
11	12	13	14	15
6	7	8	9	10
1	2	3	4	5

Proc 0   Proc 1
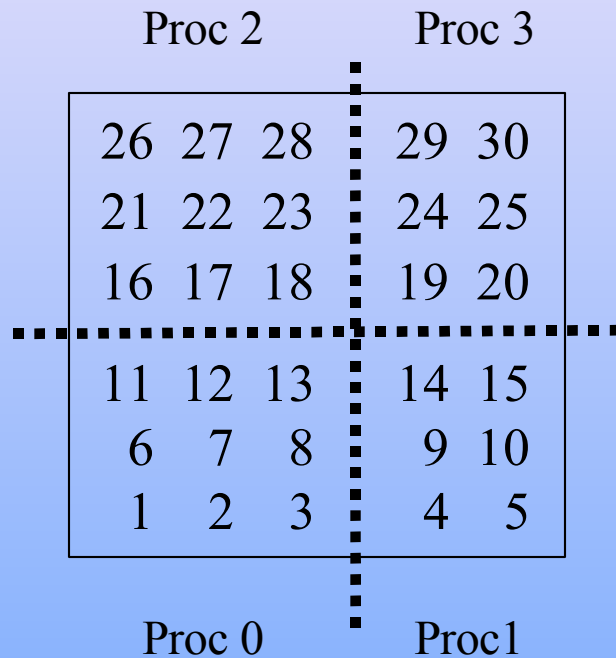
Natural numbering, corresponding
to the entire problem domain

Proc 2   Proc 3

22	23	24	29	30
19	20	21	27	28
16	17	18	25	26
7	8	9	14	15
4	5	6	12	13
1	2	3	10	11

Proc 0   Proc 1

PETSc numbering used by DAs

data layout:
distributed arrays

Mapping Between Global Numberings

- Natural global numbering
  - convenient for visualization of global problem, specification of certain boundary conditions, etc.

- Can convert between various global numbering schemes using AO (Application Orderings)
  - DAGetAO(DA da, AO *ao);
  - AO usage explained in next section

- Some utilities (e.g., VecView()) automatically handle this mapping for global vectors attained from DAs

data layout:
distributed arrays

Distributed Array Example

- Files: src/snes/examples/tutorial/ex5.c, ex5f.F
  - Functions that construct vectors and matrices use a naturally associated DA
    - DAGetMatrix()
    - DASetLocalFunction()
    - DASetLocalJacobian()

data layout:
distributed arrays

The Bratu Equation I
SNES Example 5

- Create SNES and DA
- Use DASetLocalFunction()
  - Similarly DASetLocalJacobian()
- Use SNESDAFormFunction() for SNES
  - Could also use FormFunctionMatlab()
- Similarly SNESDAComputeJacobian()
  - Use DAGetMatrix() for SNES Jacobian
  - Could also use SNESDefaultComputeJacobian()

The Bratu Equation II
SNES Example 5

- int FormFunctionLocal(DALocalInfo *info,

    PetscScalar **x, PetscScalar **f,

    void *ctx)

```
for(j = info->ys; j < info->ys + info->ym; j++) {
  for(i = info->xs; i < info->xs + info->xm; i++) {
    if (i == 0 || j == 0 || i == info->mx-1 || j == info->my-1) {
      f[j][i] = x[j][i];
    } else {
      u       = x[j][i];
      u_xx    = -(x[j][i+1] - 2.0*u + x[j][i-1])*(hy/hx);
      u_yy    = -(x[j+1][i] - 2.0*u + x[j-1][i])*(hx/hy);
      f[j][i] = u_xx + u_yy - hx*hy*lambda*PetscExpScalar(u);
    }
  }
}
```

The Bratu Equation III
SNES Example 5

- int FormJacobianLocal(DALocalInfo *info, PetscScalar **x,

  Mat jac, void *ctx)

```
for(j = info->ys; j < info->ys + info->ym; j++) {
  for(i = info->xs; i < info->xs + info->xm; i++) {
    row.j = j; row.i = i;
    if (i == 0 || j == 0 || i == info->mx-1 || j == info->my-1) {
      v[0] = 1.0;
      MatSetValuesStencil(jac,1,&row,1,&row,v,INSERT_VALUES);
    } else {
      v[0] = -(hx/hy); col[0].j = j-1; col[0].i = i;
      v[1] = -(hy/hx); col[1].j = j;   col[1].i = i-1;
      v[2] = 2.0*(hy/hx+hx/hy) - hx*hy*lambda*PetscExpScalar(x[j][i]);
      v[3] = -(hy/hx); col[3].j = j;   col[3].i = i+1;
      v[4] = -(hx/hy); col[4].j = j+1; col[4].i = i;
      MatSetValuesStencil(jac,1,&row,5,col,v,INSERT_VALUES);
    }
  }
}
```

137

VecScatter: Vector Scatters & Gathers

Parallel data layout and ghost values for unstructured meshes

intermediate

intermediate

intermediate

intermediate

intermediate

- Mapping between global numberings

- Local and global indices

- VecScatter creation

- Ghost point updates

- Setting object data using local indices

tutorial outline:
data layout:
vector scatters

Unstructured Meshes

- Setting up communication patterns is much more complicated than the structured case due to
    - mesh dependence
    - discretization dependence

beginner

data layout:
vector scatters

Sample Differences Among Discretizations

- Cell-centered

- Vertex-centered

- Cell and vertex centered (e.g., staggered grids)

- Mixed triangles and quadrilaterals

beginner

data layout:
vector scatters

Unstructured Mesh Concepts

- AO: Application Orderings
  - map between various global numbering schemes
- IS: Index Sets
  - indicate collections of nodes, cells, etc.
- VecScatter:
  - update ghost points using vector scatters/gathers
- ISLocalToGlobalMapping
  - map from a local (on-processor) numbering of indices to a global (across-processor) numbering

intermediate

data layout:
vector scatters

Communication and Physical Discretization: Unstructured Meshes

Communication	Local Numerical Computation

Geometric Data Data Structure Creation Ghost Point Data Structures Ghost Point Updates

elements
edges
vertices

VecScatterCreate( )

VecScatter
AO

VecScatter( )

Loops over entities

unstructured meshes
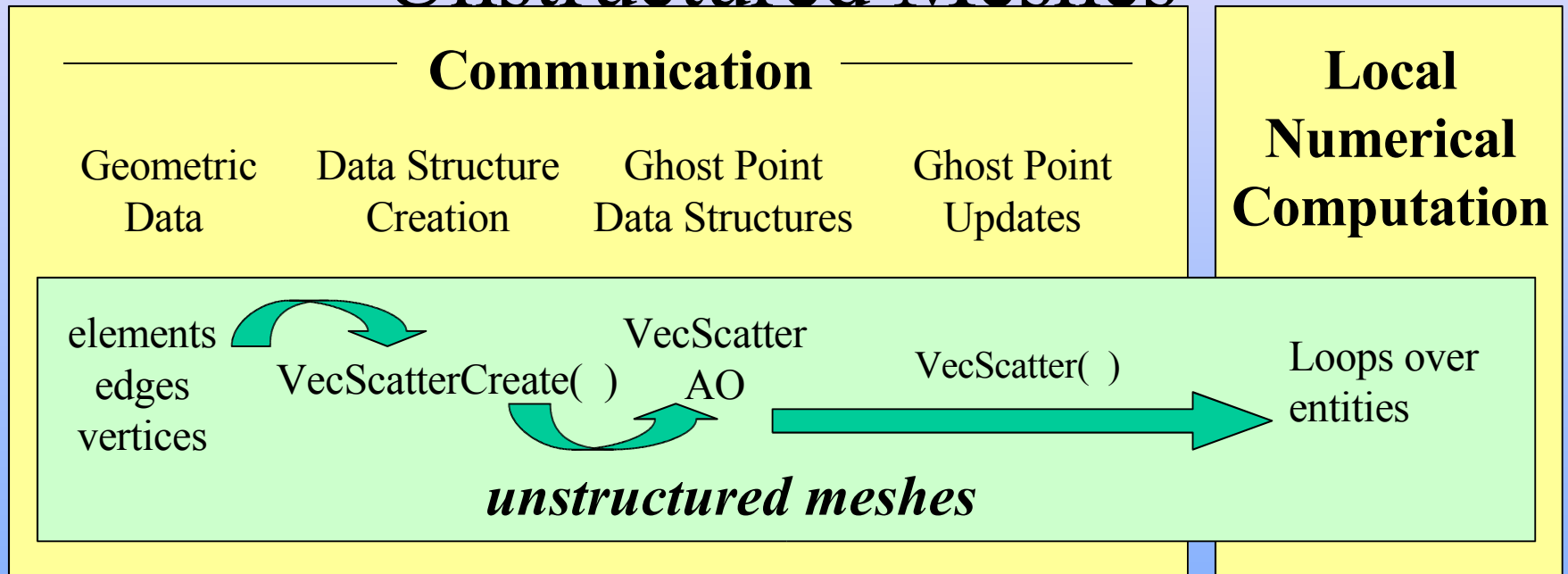
intermediate

data layout:
vector scatters

Setting Up the Communication Pattern
(the steps in creating VecScatter)

- Renumber objects so that contiguous entries are adjacent (AO)

- Determine needed neighbor values

- Generate local numbering

- Generate local and global vectors

- Create communication object (VecScatter)

intermediate

data layout:
vector scatters

Cell-based Finite Volume
Application Numbering
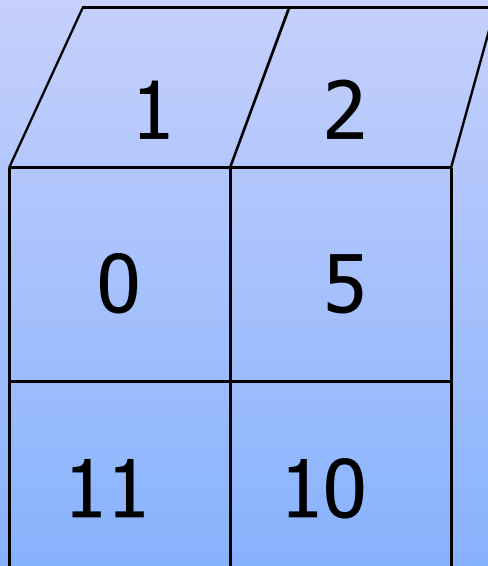
Proc 0   Proc1
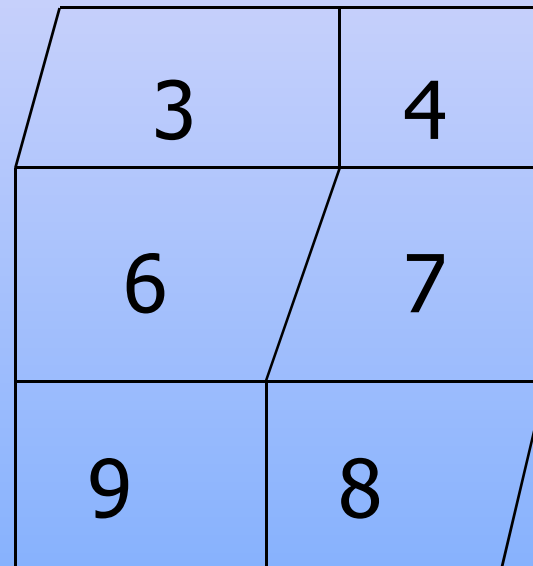
global indices defined by application

intermediate
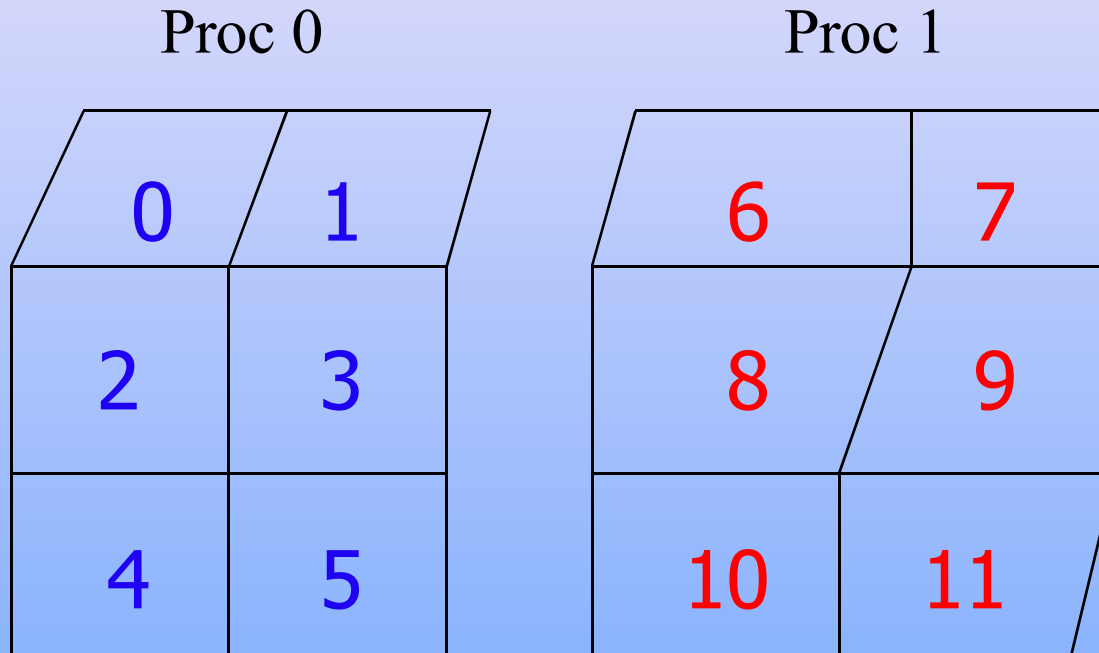
data layout:
vector scatters

Remapping Global Numbers: An Example

- Processor 0
  - nlocal: 6
  - app_numbers: {1,2,0,5,11,10}
  - petsc_numbers: {0,1,2,3,4,5}

- Processor 1
  - n_local: 6
  - app_numbers: {3,4,6,7,9,8}
  - petsc_numbers: {6,7,8,9,10,11}

Proc 0   Proc 1

PETSc numbers

0	1		6	7
2	3		8	9
4	5		10	11

application numbers

1	2		3	4
0	5		6	7
11	10		9	8
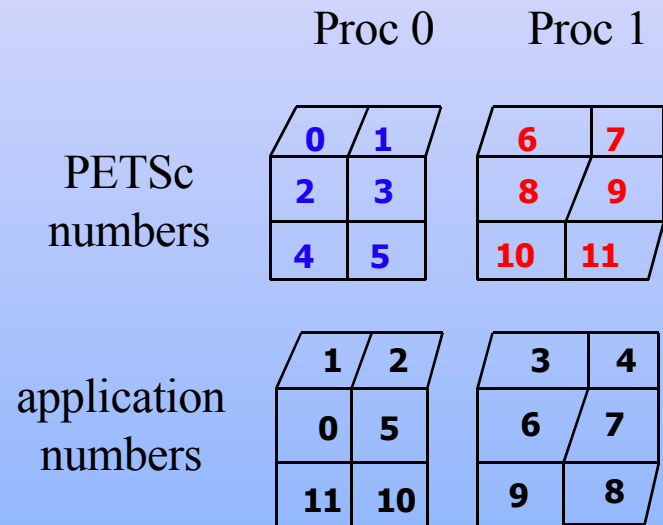
intermediate

data layout: vector scatters

Remapping Numbers (1)

- Generate a parallel object (AO) to use in mapping between numbering schemes

- AOCreateBasic(MPI_Comm comm,
  - int nlocal,
  - int *app_numbers,
  - int *petsc_numbers,
  - AO *ao);

intermediate

data layout:
vector scatters

Remapping Numbers (2)

- AOApplicationToPetsc(AO *ao,
  - int number_to_convert,
  - int *indices);

- For example, if $indices[\,]$ contains the cell neighbor lists in an application numbering, then apply AO to convert to new numbering

intermediate

data layout:
vector scatters

Neighbors

using global PETSc numbers

Proc 0

Proc1

0	1	6
2	3	8
4	5	10

1	6	7
3	8	9
5	10	11
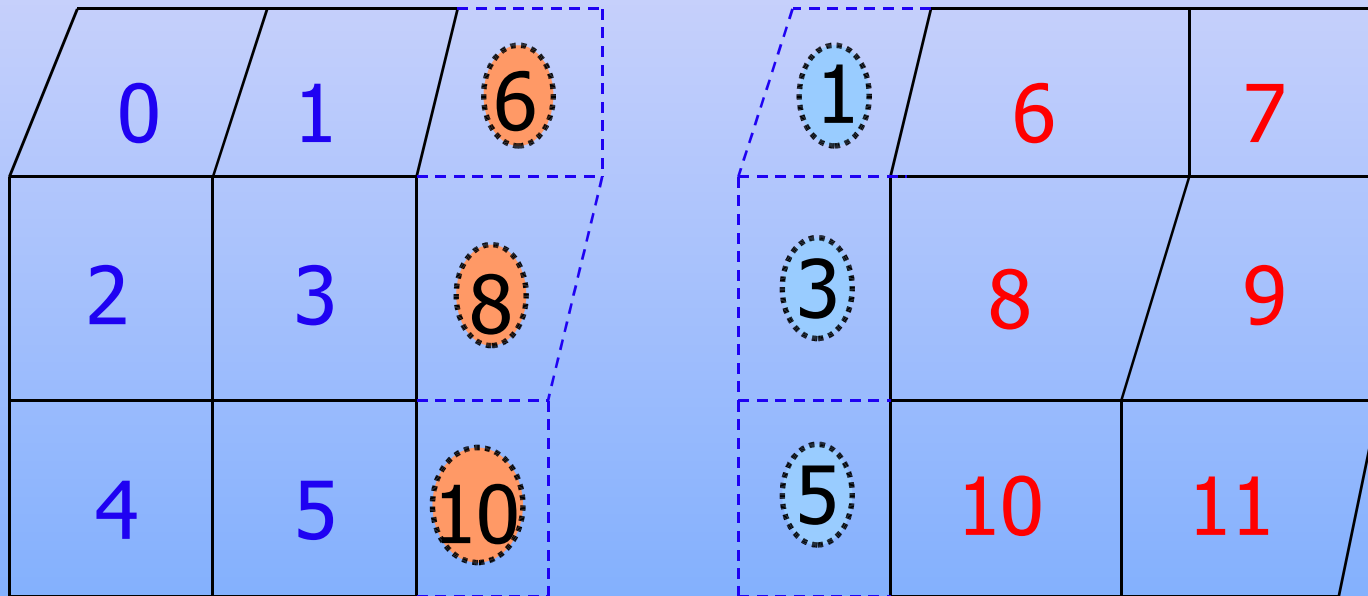
ghost cells

intermediate

data layout:
vector scatters

Local Numbering

Proc 0

Proc1

0   1   **6**

2   3   **7**

4   5   **8**

6   0   1

7   2   3

8   4   5
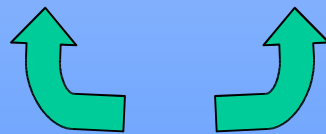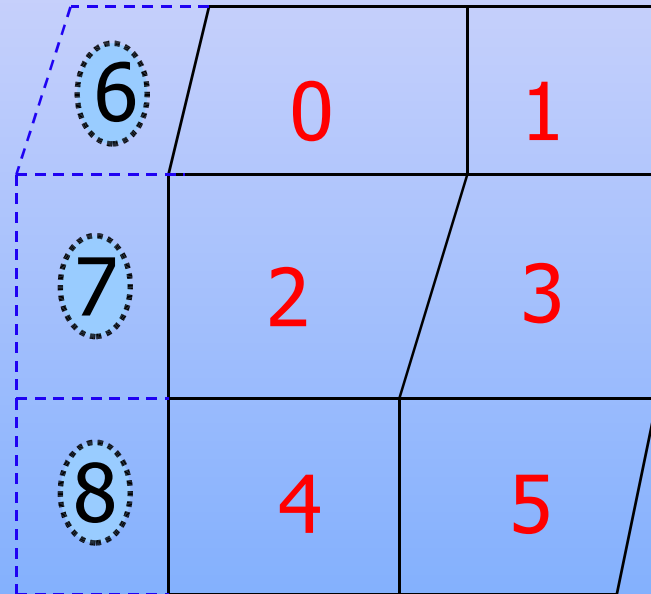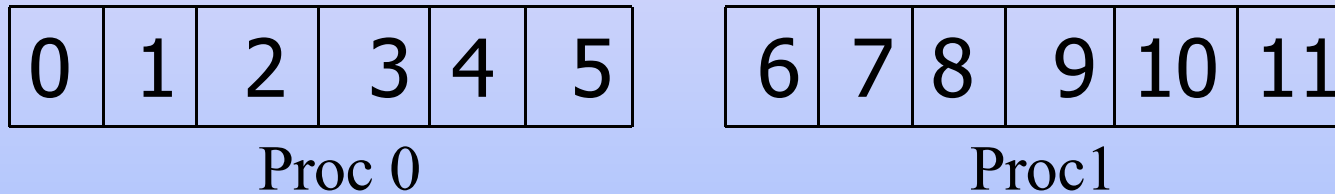
ghost cells

intermediate

data layout:
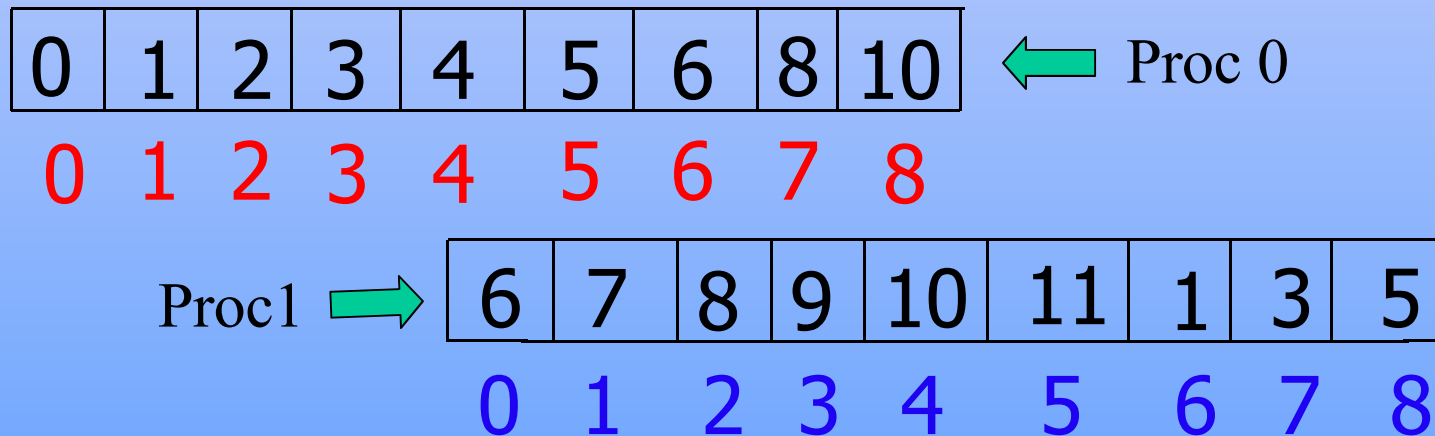vector scatters

Global and Local Representations

- Global representation

  - parallel vector with no ghost locations

  - suitable for use by PETSc parallel solvers

- Local representation

  - sequential vectors with room for ghost points

  - used to evaluate functions, Jacobians, etc.

intermediate

data layout:
vector scatters

Creating Vectors

- Sequential

  VecCreateSeq(PETSC_COMM_SELF,

  9,Vec *lvec);

- Parallel

  VecCreateMPI(PETSC_COMM_WORLD,

  6,PETSC_DETERMINE,Vec *gvec)

intermediate

data layout:
vector scatters

Local and Global Indices

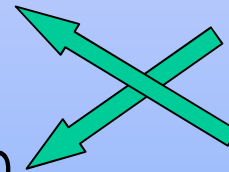- ## Processor 0
  - ISCreateGeneral(PETSC_COMM_WORLD,
    9,{0,1,2,3,4,5,6,8,10},IS *isg);
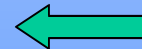 - ISCreateStride(PETSC_COMM_SELF,
    9,0,1,IS* isl);

ISCreateGeneral() - Specify *global* numbers of locally owned cells, including ghost cells

- ## Processor 1
  - ISCreateGeneral(PETSC_COMM_WORLD,
    9,{6,7,8,9,10,11,1,3,5},IS *isg);
  - ISCreateStride(PETSC_COMM_SELF,
    9,0,1,IS* isl);

ISCreateStride() - Specify *local* numbers of locally owned cells, including ghost cells

intermediate

data layout: vector scatters

Creating Communication Objects

- VecScatterCreate(Vec gvec,
  - IS gis,
  - Vec lvec,
  - IS lis
  - VecScatter gtol);
- Determines all required messages for mapping data from a global vector to local (ghosted) vectors

intermediate

data layout:
vector scatters

Performing a Global-to-Local Scatter

Two-step process that enables overlapping computation and communication

- VecScatterBegin(VecScatter gtol,
  - Vec gvec,
  - Vec lvec,
  - INSERT_VALUES
  - SCATTER_FORWARD);
- VecScatterEnd(...);

intermediate

data layout:
vector scatters

Performing a Local-to-Global Scatter

- VecScatterBegin(VecScatter gtol,
  - Vec lvec,
  - Vec gvec,
  - ADD_VALUES,
  - SCATTER_REVERSE);
- VecScatterEnd(...);

data layout:
vector scatters

Setting Values in Global Vectors and Matrices using a Local Numbering

- Create mapping
  - ISLocalToGlobalMappingCreateIS(IS gis, ISLocalToGlobalMapping *lgmap);
- Set mapping
  - VecSetLocalToGlobalMapping(Vec gvec, ISLocalToGlobalMapping lgmap);
  - MatSetLocalToGlobalMapping(Mat gmat, ISLocalToGlobalMapping lgmap);
- Set values with local numbering
  - VecSetValuesLocal(Vec gvec,int ncols, int localcolumns, Scalar *values, …);
  - MatSetValuesLocal(Mat gmat, ...);
  - MatSetValuesLocalBlocked(Mat gmat, ...);

intermediate

data layout:
vector scatters

Sample Function Evaluation

```
int FormFunction(SNES snes, Vec Xglobal, Vec Fglobal, void *ptr)
{
    AppCtx  *user = (AppCtx *) ptr;
    double   x1, x2, f1, f2, *x, *f ;
    int        *edges = user->edges;

    VecScatterBegin(user->scatter, Xglobal, Xlocal, SCATTER_FORWARD, INSERT_VALUES);
    VecScatterEnd(user->scatter, Xglobal, Xlocal, SCATTER_FORWARD, INSERT_VALUES);

    VecGetArray(Xlocal,&X);   VecGetArray(Flocal,&F);
    for (i=0; i < user->nlocal; i++)  {
        x1 = X[edges[2*i]];  x2 = X[edges[2*i+1]];  /* then compute f1, f2 */
        F[edges[2*i]] += f1;  F[edges[2*i+1]] += f2;
    }
    VecRestoreArray(Xlocal,&X);   VecRestoreArray(Flocal,&F);

    VecScatterBegin(user->scatter, Flocal, Fglobal, SCATTER_REVERSE, INSERT_VALUES);
    VecScatterEnd(user->scatter, Flocal, Fglobal, SCATTER_REVERSE, INSERT_VALUES);
    return 0;
}
```
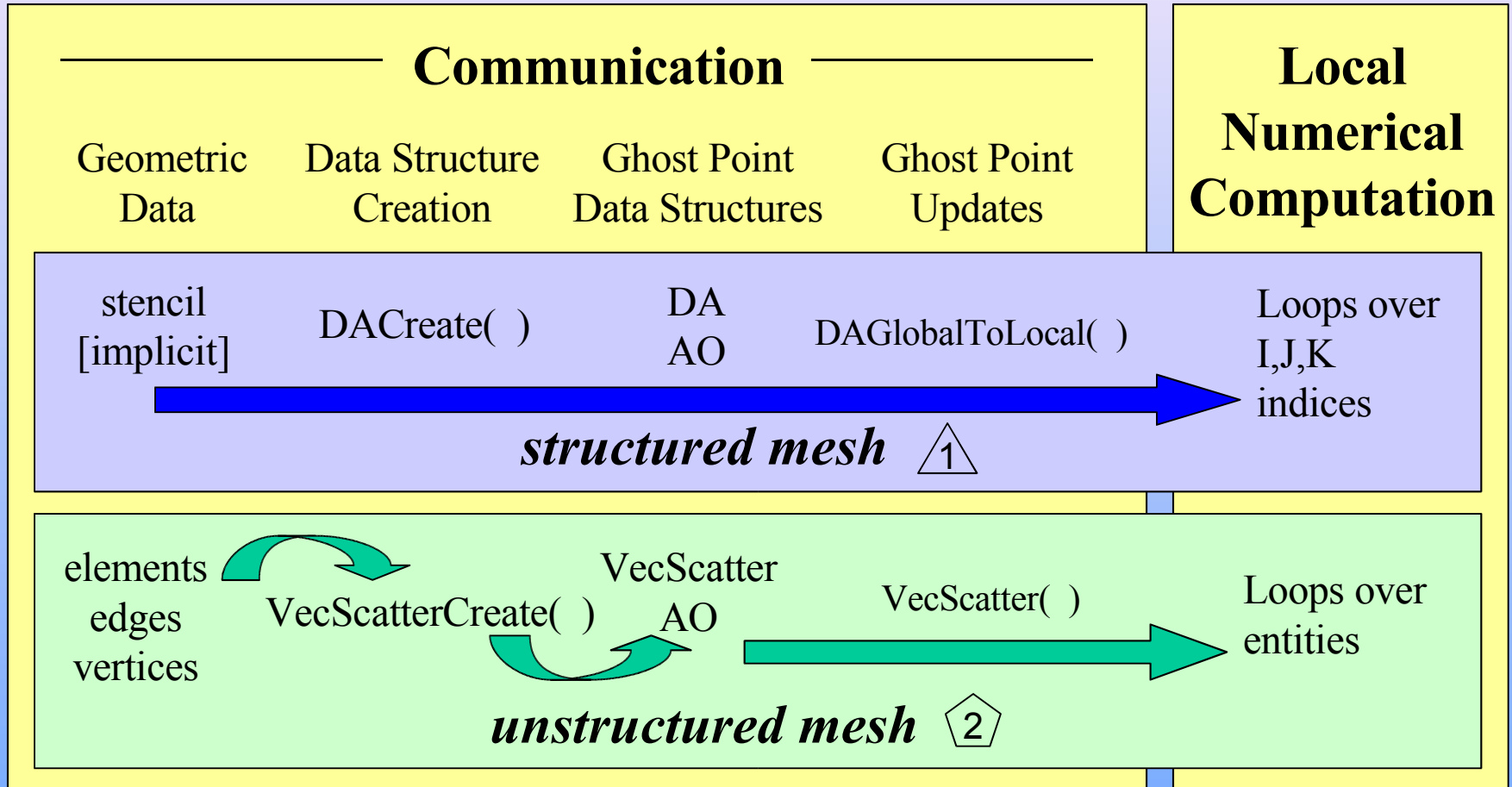
intermediate

data layout:
vector scatters

Communication and Physical Discretization

	Communication			**Local Numerical Computation**
Geometric Data	Data Structure Creation	Ghost Point Data Structures	Ghost Point Updates	

structured mesh △1

stencil [implicit]   DACreate( )   DA AO   DAGlobalToLocal( )   Loops over I,J,K indices

unstructured mesh ⬠2

elements edges vertices   VecScatterCreate( )   VecScatter AO   VecScatter( )   Loops over entities

△1 beginner | ⬠2 intermediate

data layout

Interfacing to 3rd party Packages

Using PETSc with Other Packages:
Linear Solvers

- ## Interface Approach
  - External linear solvers typically use a variant of CSR matrix
  - Each package has a matrix subclass with overridden methods

- ## Usage
  - Set preconditioners via the usual approach
    - Procedural interface: PCSetType(pc,"spai")
    - Runtime option: -pc_type spai
  - Set preconditioner-specific options via the usual approach
    - PCSPAISetEpsilon(), PCSPAISetVerbose(), etc.
    - -pc_spai_epsilon <eps>   -pc_spai_verbose etc.

Using PETSc with Other Packages:
HYPRE - Preconditioners

- ## Several preconditioners
  - -pc_type hypre
  - -pc_hypre_type [pilut,parasails,boomeramg,euclid]

- ## Specialize preconditioner
  - -pc_hypre_boomeramg_max_levels <num>
  - -pc_hypre_boomeramg_grid_sweeps <fine,down,up,coarse>

- ## Options can be displayed with -help
  - Only for selected types

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

- 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) – uses a similar interface approach

- **TAO** is evolving toward
  - CCA-compliant component-based design (see http://www.cca-forum.org)

TAO Interface

```
TAO_SOLVER    tao;                    /*  optimization solver  */
Vec               x, g;                    /*  solution and gradient vectors  */
ApplicationCtx    usercontext;         /*  user-defined context  */

TaoInitialize();

/* Initialize Application -- Create variable and gradient vectors x and g */   ...

TaoCreate(MPI_COMM_WORLD,"tao_lmvm",&tao);
TaoSetFunctionGradient(tao,x,g, FctGrad,(void*)&usercontext);

TaoSolve(tao);

/* Finalize application -- Destroy vectors x and g */   ...

TaoDestroy(tao);
TaoFinalize();
```

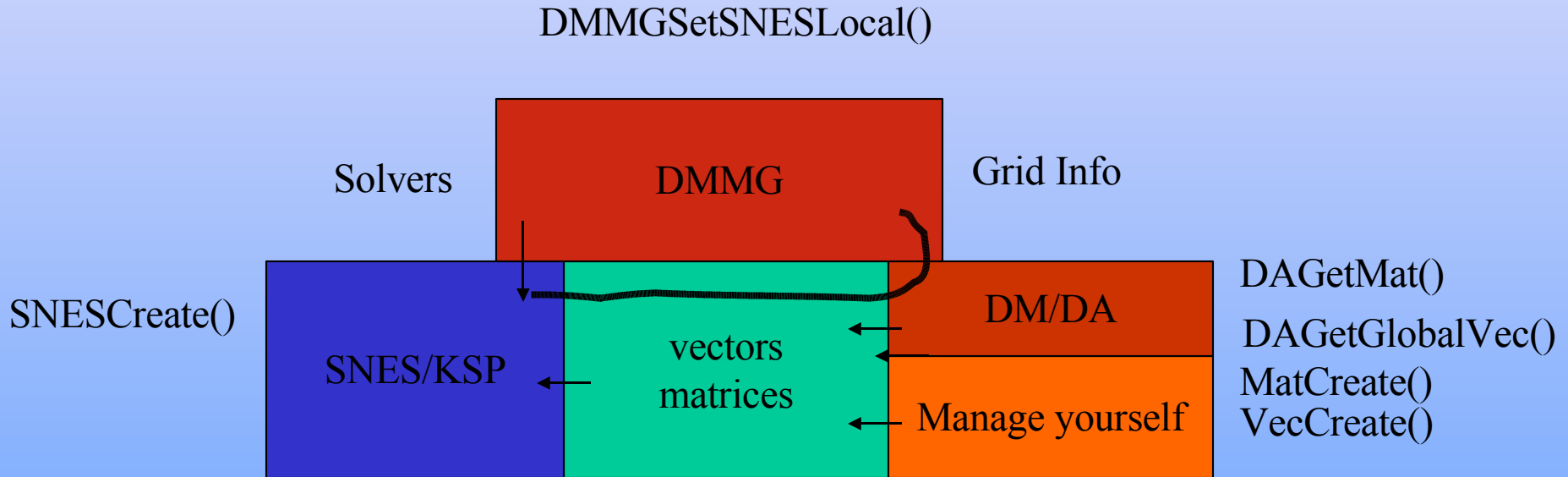Similar Fortran interface, e.g., call TaoCreate(...)

software
interfacing:
TAO

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 allows C/Fortran programmers to use Matlab functions
    - PetscMatlabEngine – unwraps PETSc vectors and matrices for MatlabEngine

- 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)

Three Ways of Using PETSc

DMMGSetSNESLocal()

Solvers

DMMG

Grid Info

SNESCreate()

SNES/KSP

vectors matrices

DM/DA

Manage yourself

DAGetMat()

DAGetGlobalVec()

MatCreate()
VecCreate()

DMMG data management multigrid

- Creates the vectors, matrices,… appropriate for your grid.

- Connects them to a (hierarchy of) solvers

- User provides "local physics"

References

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