PETSc

Portable, Extensible Toolkit for Scientific Computation

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Freelance Computational Scientist

Workshop on Modern Scientific Computing

DTU Compute, Technical University of Denmark

March 2-3, 2016

Introducing Myself

Education

Master's Degrees in Microelectronics and Mathematics

Doctoral Degree in Microelectronics

Home University: TU Wien

Interests

Efficient Numerics on Modern Hardware

High-level APIs

Semiconductor Device Simulation

Contact

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Web: http://www.karlrupp.net/

Find me at: Google+, Twitter, LinkedIn

Before we start...

Goal of this Workshop

You should learn new things about HPC

Ask Questions

Tell me if you do not understand

Ask for further details

Don’t be shy

Schedule for Day 1

Morning: Lecture

- About PETSc
- Vectors and matrices
- Linear solvers and preconditioners
- Distributed arrays

Afternoon: Hands-On

- PETSc configuration and installation
- Debugging your PETSc code
- Step-by-step implementation of a scalable Poisson solver
- Experimentation with preconditioners

About PETSc

PETSc Origins

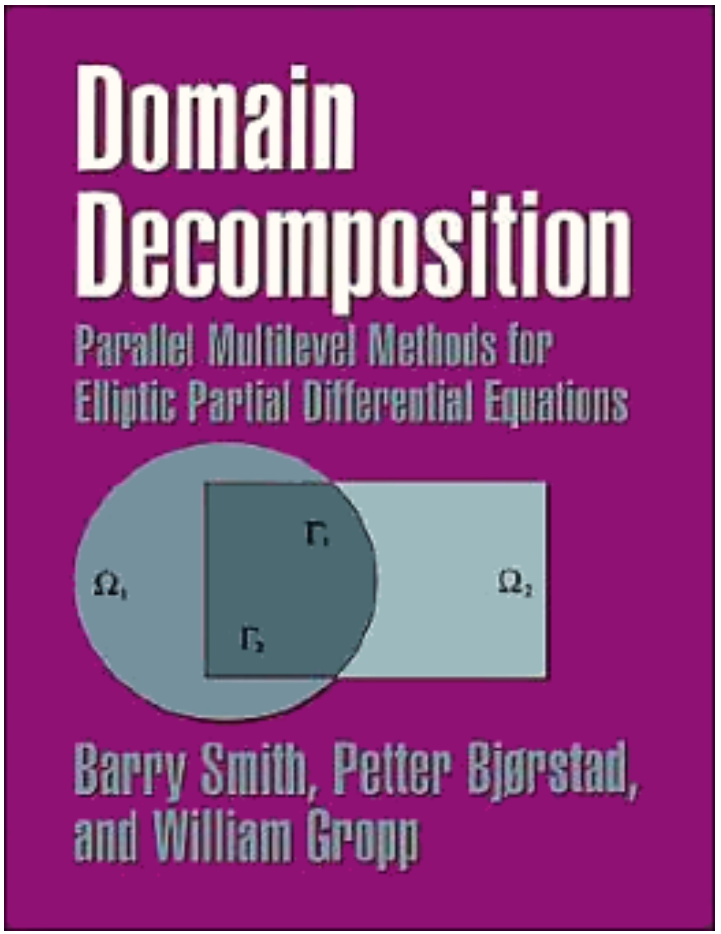
PETSc was developed as a Platform for

Experimentation

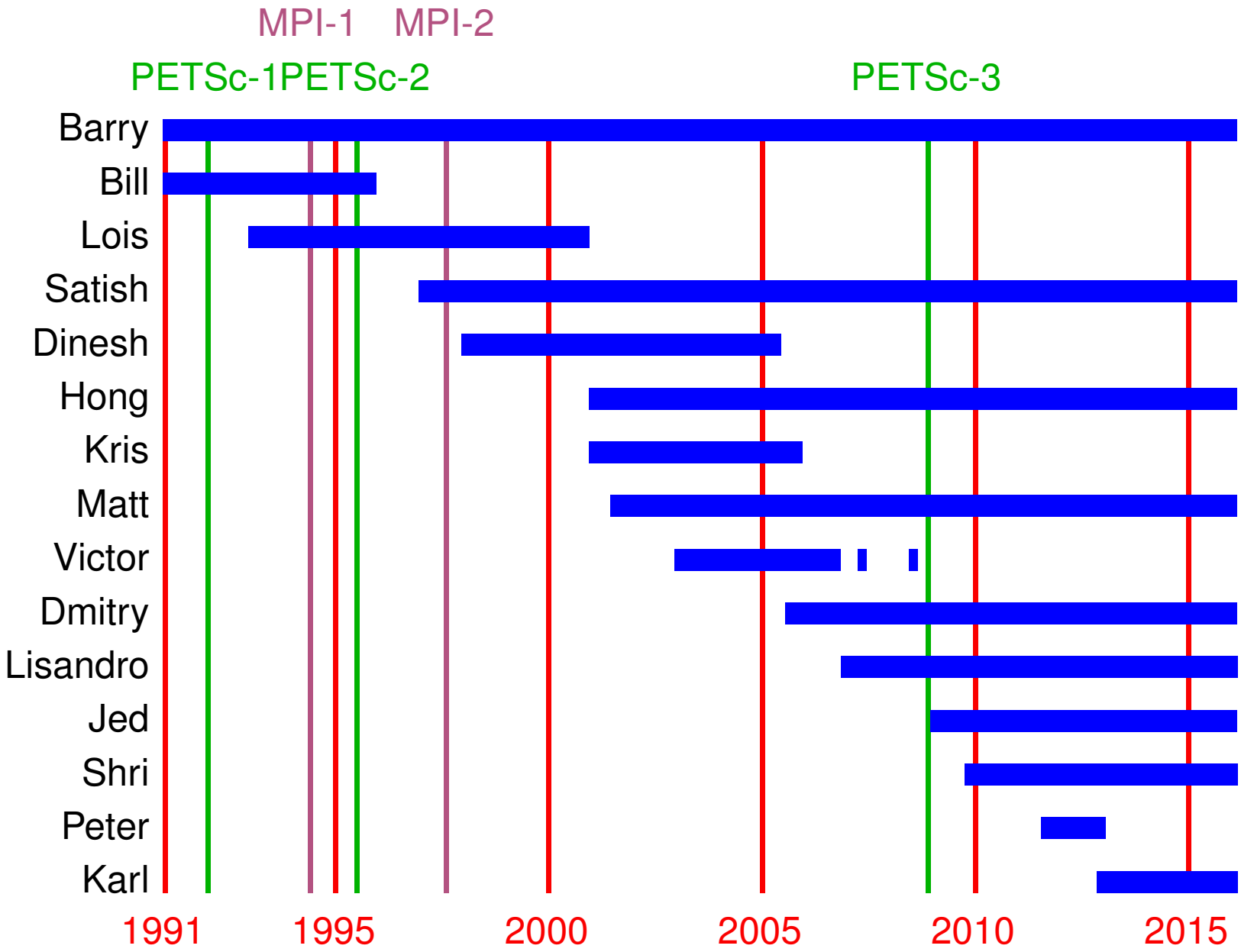
We want to experiment with different

- Models
- Discretizations
- Solvers
- Algorithms

These boundaries are often blurred...



Timeline


MPI-1
MPI-2
PETSc-1PETSc-2
PETSc-3
Barry
Bill
Lois
Satish
Dinesh
Hong
Kris
Matt
Victor
Dmitry
Lisandro
Jed
Shri
Peter
Karl
1991
1995
2000
2005
2010
2015

PETSc

Portable Extensible Toolkit for Scientific Computing

Architecture

tightly coupled (e.g. XT5, BG/P, Earth Simulator)

loosely coupled such as network of workstations

GPU clusters (many vector and sparse matrix kernels)

Software Environment

Operating systems (Linux, Mac, Windows, BSD, proprietary Unix)

Any compiler

Usable from C, C++, Fortran 77/90, Python, and MATLAB

Real/complex, single/double/quad precision, 32/64-bit int

System Size

500B unknowns, 75% weak scalability on Jaguar (225k cores) and Jugene (295k cores)

Same code runs performantly on a laptop

Free to everyone (BSD-style license), open development

PETSc

Portable **Extensible** Toolkit for Scientific Computing

Philosophy: Everything has a plugin architecture

Vectors, Matrices, Coloring/ordering/partitioning algorithms

Preconditioners, Krylov accelerators

Nonlinear solvers, Time integrators

Spatial discretizations/topology

Example

Vendor supplies matrix format and associated preconditioner, distributes compiled shared library.

Application user loads plugin at runtime, no source code in sight.

PETSc

Portable Extensible **Toolkit** for Scientific Computing

Toolset

algorithms

(parallel) debugging aids

low-overhead profiling

Composability

try new algorithms by choosing from product space

composing existing algorithms (multilevel, domain decomposition, splitting)

Experimentation

Impossible to pick the solver *a priori*

PETSc's response: expose an algebra of composition

keep solvers decoupled from physics and discretization

PETSc

Portable Extensible Toolkit for **Scientific Computing**

Computational Scientists

PyLith (CIG), Underworld (Monash), Magma Dynamics (LDEO, Columbia), PFLOTRAN (DOE), SHARP/UNIC (DOE)

Algorithm Developers (iterative methods and preconditioning)

Package Developers

SLEPc, TAO, Deal.II, Libmesh, FEniCS, PETSc-FEM, MagPar, OOFEM, FreeCFD, OpenFVM

Funding

Department of Energy

SciDAC, ASCR ISICLES, MICS Program, INL Reactor Program

National Science Foundation

CIG, CISE, Multidisciplinary Challenge Program

Documentation and Support

Hundreds of tutorial-style examples

Hyperlinked manual, examples, and manual pages for all routines

Support from `petsc-maint@mcs.anl.gov`

The Role of PETSc

Developing parallel, nontrivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.

PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver, nor a silver bullet.

— Barry Smith

Obtaining PETSc

Linux Package Managers

Web: http://mcs.anl.gov/petsc, download tarball

Git: https://bitbucket.org/petsc/petsc

Mercurial: https://bitbucket.org/petsc/petsc-hg

Installing PETSc

```
$> cd /path/to/petsc/workdir
$> git clone https://bitbucket.org/petsc/petsc.git \
     --branch master --depth 1
$> cd petsc
```

```
$> export PETSC_DIR=$PWD PETSC_ARCH=mpich-gcc-dbg
$> ./configure --with-cc=gcc --with-fc=gfortran
     --download-fblaslapack --download-{mpich,ml,hypre}
```

PETSc External Packages

Most packages can be automatically

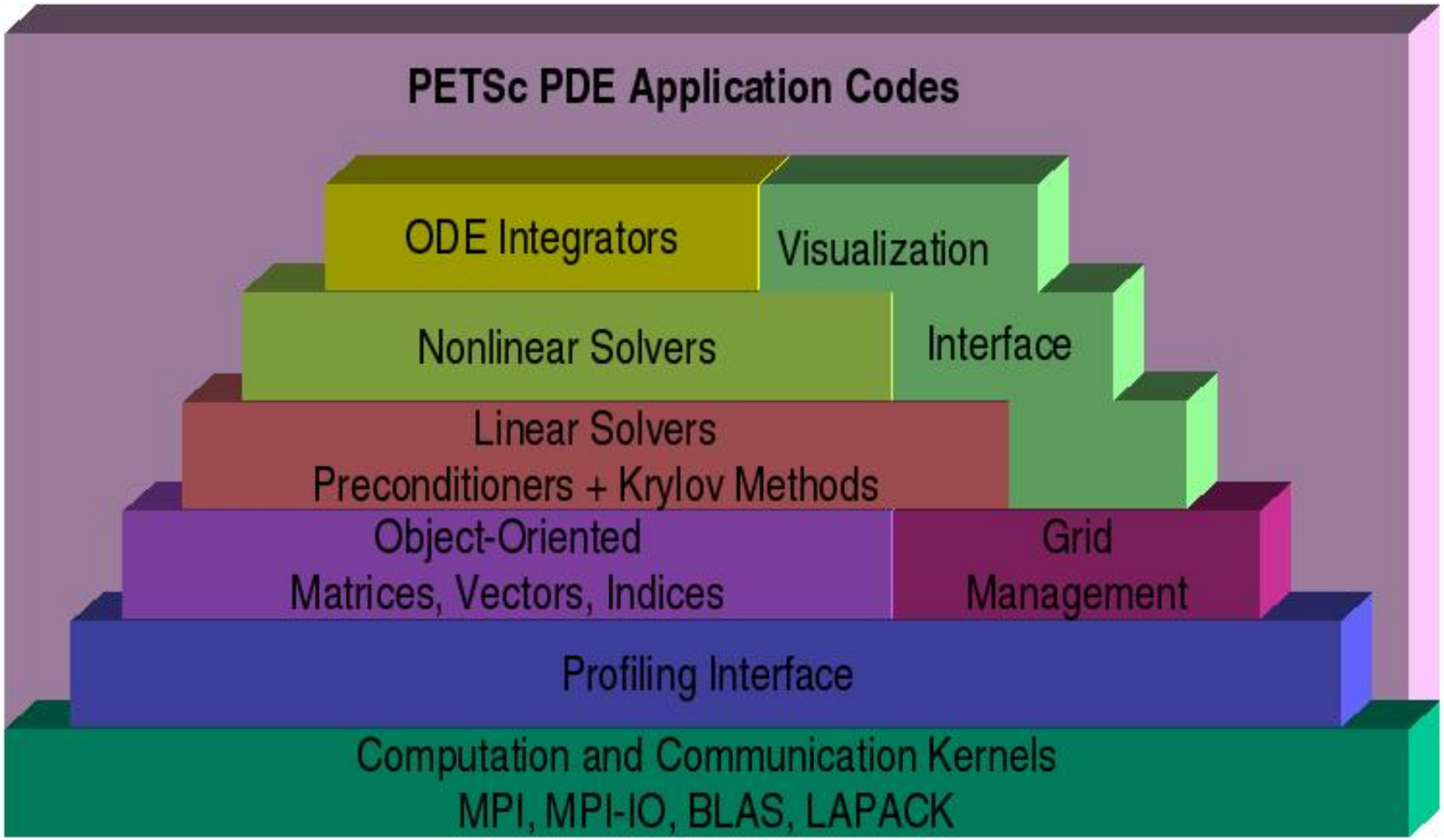
- Downloaded
- Configured and Built (in `$PETSC_DIR/externalpackages`)
- Installed with PETSc

Works for (list incomplete)

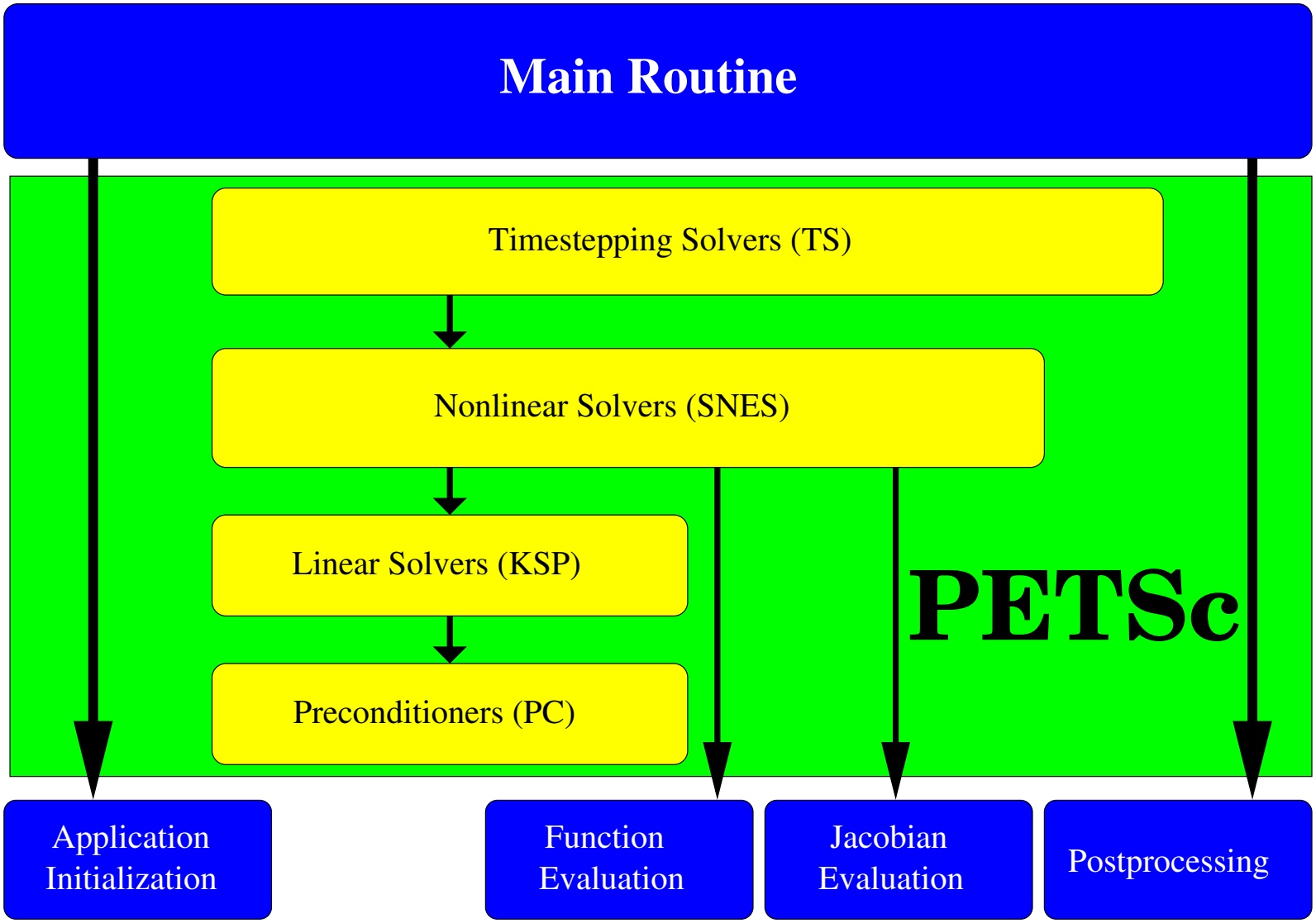
- petsc4py
- PETSc documentation utilities (Sowing, lgrind, c2html)
- BLAS, LAPACK, BLACS, ScaLAPACK, PLAPACK
- MPICH, MPE, OpenMPI
- ParMetis, Chaco, Jostle, Party, Scotch, Zoltan
- MUMPS, Spooles, SuperLU, SuperLU_Dist, UMFPack, pARMS
- PaStiX, BLOPEX, FFTW, SPRNG
- Prometheus, HYPRE, ML, SPAI
- Sundials
- Triangle, TetGen, FIAT, FFC, Generator
- HDF5, Boost

PETSc Pyramid

PETSc Structure



Flow Control for a PETSc Application



Vectors and Matrices

The Role of PETSc

You want to think about how you decompose your data structures, how you think about them globally. [...]

If you were building a house, you'd start with a set of blueprints that give you a picture of what the whole house looks like. You wouldn't start with a bunch of tiles and say. "Well I'll put this tile down on the ground, and then I'll find a tile to go next to it."

But all too many people try to build their parallel programs by creating the smallest possible tiles and then trying to have the structure of their code emerge from the chaos of all these little pieces. You have to have an organizing principle if you're going to survive making your code parallel.

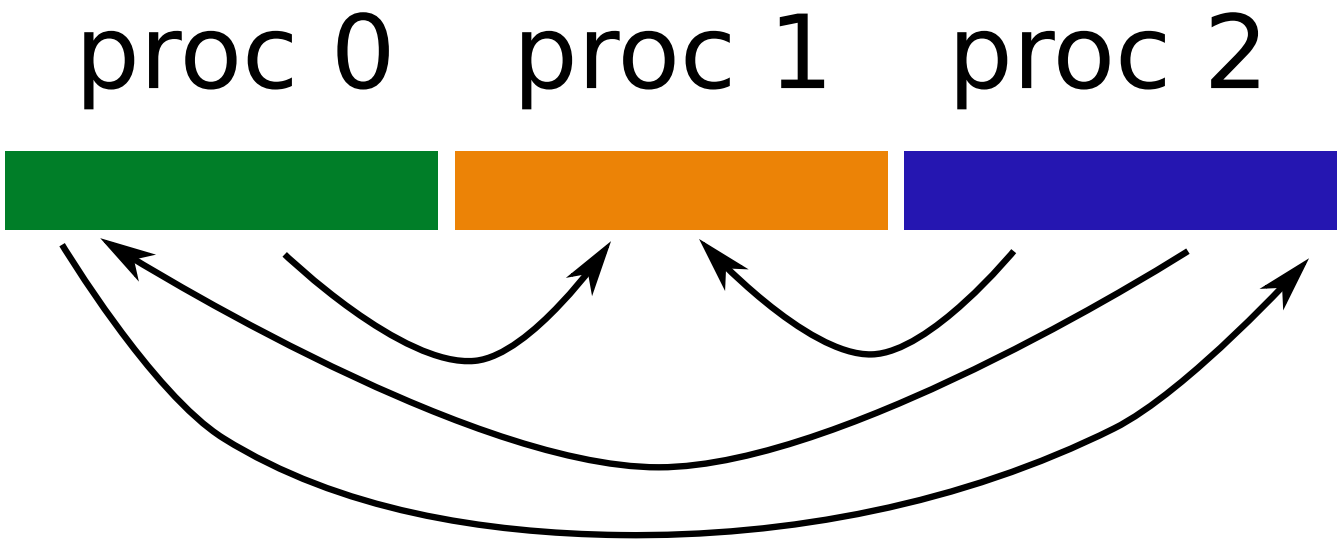
— Bill Gropp
— http://www.rce-cast.com/Podcast/rce-28-mpich2.html

PETSc Vectors

Parallel Vector Layout

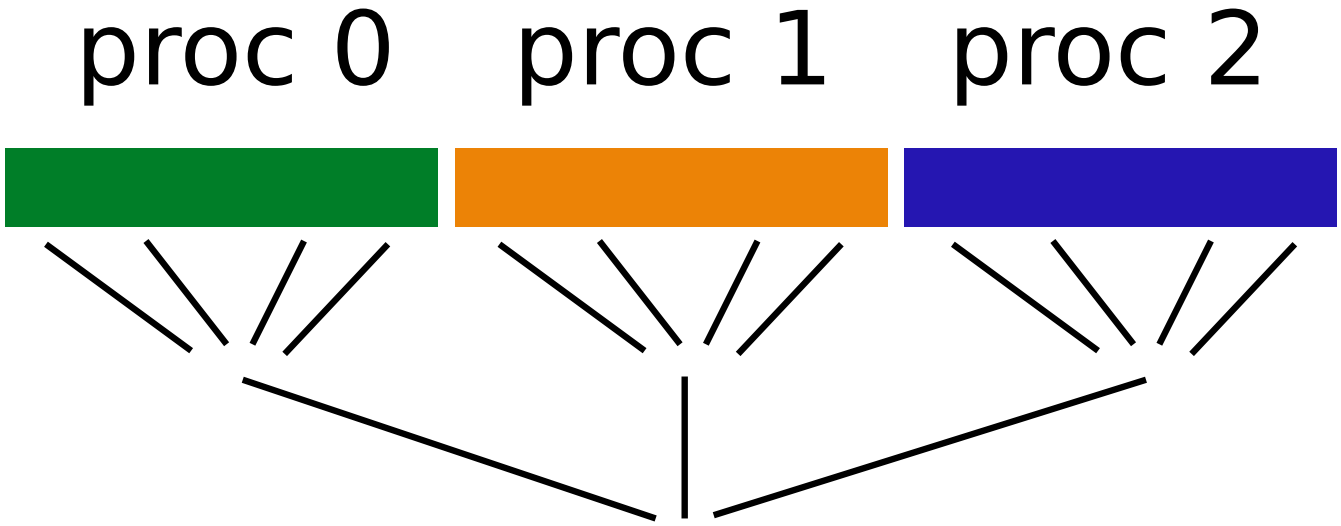

```
VecCreate(PETSC_COMM_WORLD, &x);
VecSetSizes(x, PETSC_DECIDE, N);
VecSetFromOptions(x);
```

Vector Gather and Scatter




```
// y[iy[i]] = x[ix[i]]
VecScatterCreate(...);
VecScatterBegin(...);
VecScatterEnd(...);
```

Vector Reductions




```
VecNorm(...);
VecDot(...);
VecMax(...);
...
```

PETSc Vectors

Local (Sequential) Operations

Executed by an arbitrary subset of MPI ranks

Usually involve `VecGetArray()/VecRestoreArray()`

Collective Operations

Must be executed by all processes in the MPI communicator

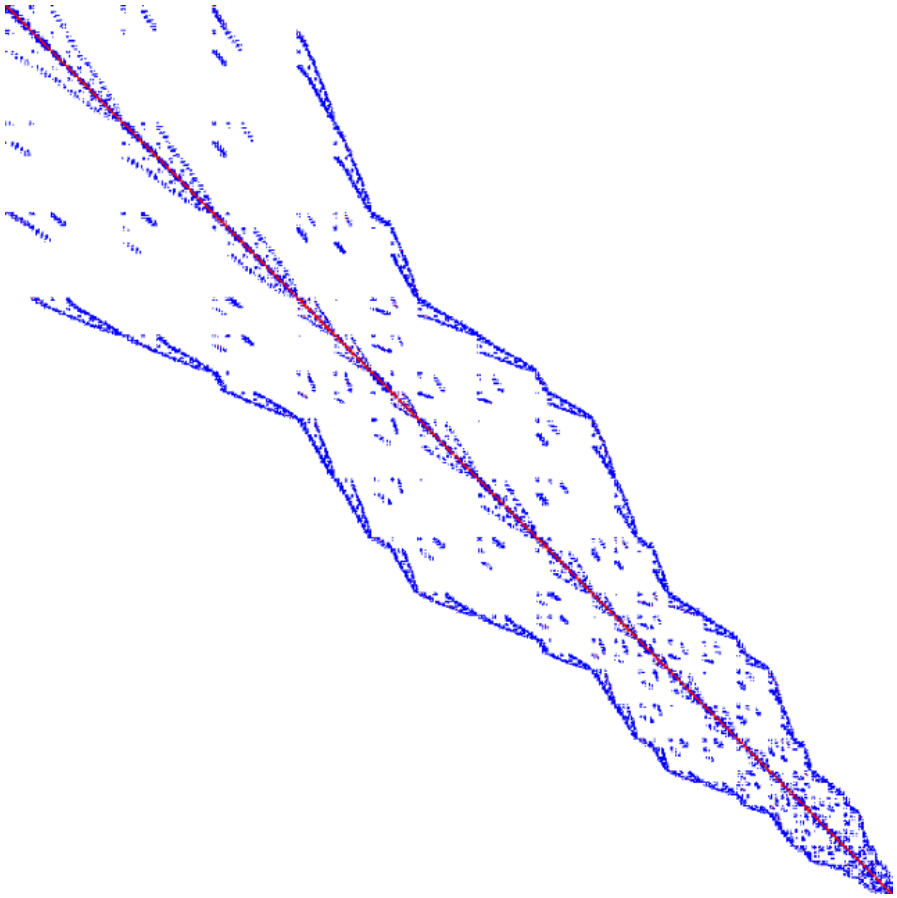
Involve MPI operations (scatter, gather, reduce, etc.)

Sparse Matrices

The important data type when solving PDEs

Two main phases:

- Filling with entries (assembly)
- Application of its action (e.g. SpMV)



Matrix Memory Preallocation

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 preallocation provides

- the freedom of dynamic data structures
- good performance

Easiest solution is to replicate the assembly code

- Remove computation, but preserve the indexing code
- Store set of columns for each row

Call preallocation routines for all datatypes

- `MatSeqAIJSetPreallocation()`
- `MatMPIBAIJSetPreallocation()`
- Only the relevant data will be used

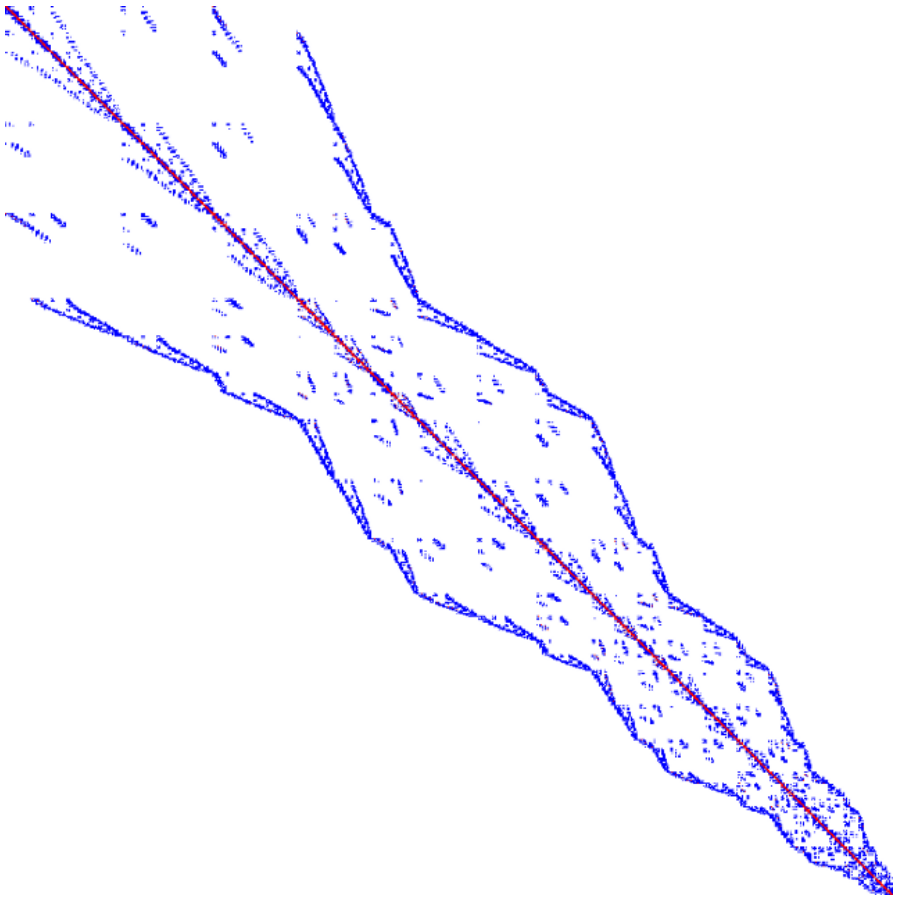
PETSc Application Integration

Sequential Sparse Matrices

```
MatSeqAIJSetPreallocation(Mat A, int nz, int nnz[])
```

nz: expected number of nonzeros in any row

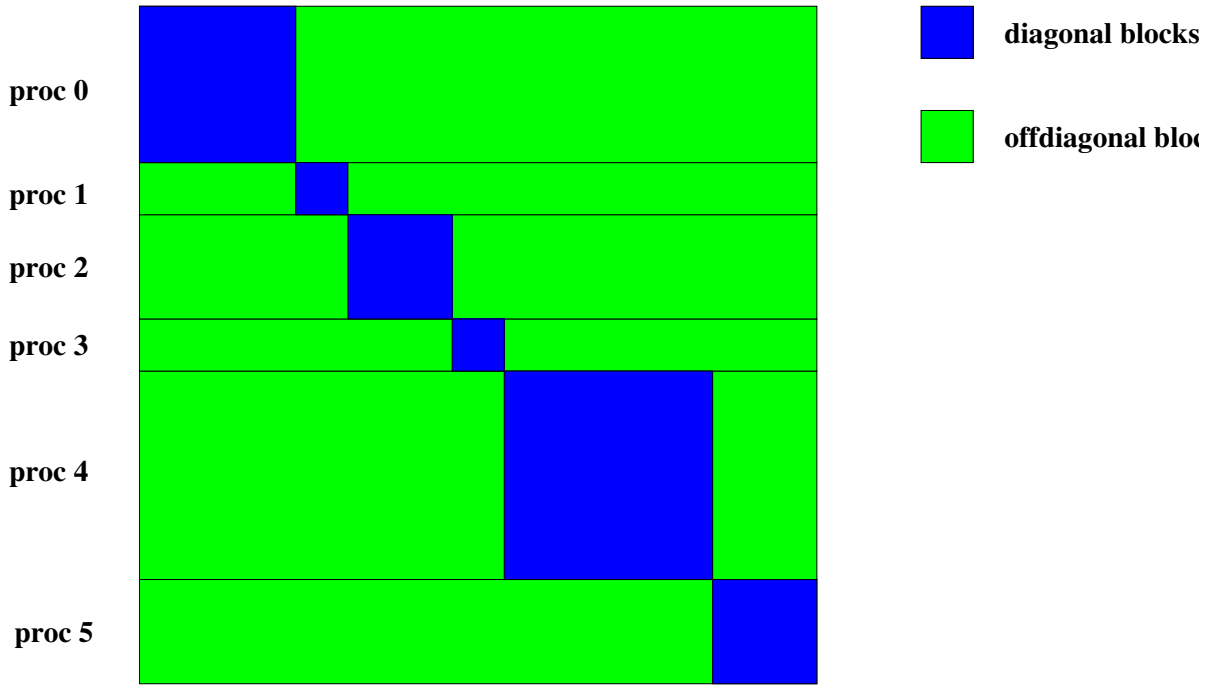
nnz(i): expected number of nonzeros in row i



Parallel Sparse Matrix

Each process locally owns a submatrix of contiguous global rows

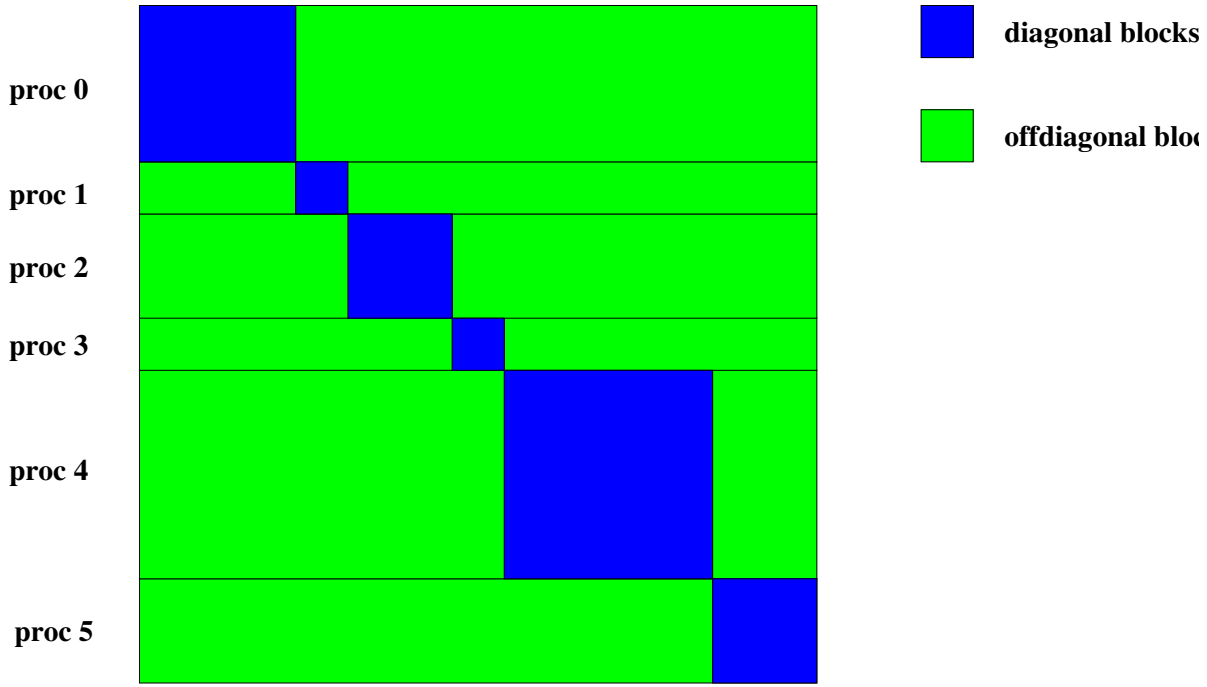
Each submatrix consists of diagonal and off-diagonal parts




```
MatGetOwnershipRange(Mat A,int *start,int *end)
```

`start`: first locally owned row of global matrix
`end-1`: last locally owned row of global matrix

PETSc Application Integration



Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
15	16	17	18	19
10	11	12	13	14
5	6	7	8	9
0	1	2	3	4
Proc 0			Proc 1	

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

PETSc numbering

PETSc Application Integration

Parallel Sparse Matrix

```
MatMPIAIJSetPreallocation(Mat A, int dnz, int dnnz[],
                                 int onz, int onnz[]
```

dnz: expected number of nonzeros in any row in the diagonal block

dnnz(i): expected number of nonzeros in row i in the diagonal block

onz: expected number of nonzeros in any row in the offdiagonal portion

onnz(i): expected number of nonzeros in row i in the offdiagonal portion

Verifying Preallocation

Use runtime options

```
-mat_new_nonzero_location_err
-mat_new_nonzero_allocation_err
```

Use runtime option

```
-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!
```

Block and Symmetric Formats

BAIJ

- Like AIJ, but uses static block size
- Preallocation is like AIJ, but just one index per block

SBAIJ

- Only stores upper triangular part
- Preallocation needs number of nonzeros in upper triangular parts of on- and off-diagonal blocks

MatSetValuesBlocked()

- Better performance with blocked formats
- Also works with scalar formats, if `MatSetBlockSize()` was called
- Variants `MatSetValuesBlockedLocal()`, `MatSetValuesBlockedStencil()`
- Change matrix format at runtime, don't need to touch assembly code

One Way to Set the Elements of a Matrix

Simple 3-point stencil for 1D Laplacian

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
if (rank == 0) {
  for(row = 0;  row < N; row++) {
    cols[0] = row-1; cols[1] = row; cols[2] = row+1;
    if (row == 0) {
      MatSetValues(A,1,&row,2,&cols[1],&v[1],
                   INSERT_VALUES);
    } else if (row == N-1) {
      MatSetValues(A,1,&row,2,cols,v,INSERT_VALUES);
    } else {
      MatSetValues(A,1,&row,3,cols,v,INSERT_VALUES);
    }
  }
}
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
```

A Better Way to Set the Elements of a Matrix

A More Efficient Way

```
v[0] = -1.0; v[1] = 2.0; v[2] = -1.0;
for(row = start;  row < end; row++) {
  cols[0] = row-1; cols[1] = row; cols[2] = row+1;
  if (row == 0) {
    MatSetValues(A,1,&row,2,&cols[1],&v[1],
                 INSERT_VALUES);
  } else if (row == N-1) {
    MatSetValues(A,1,&row,2,cols,v,INSERT_VALUES);
  } else {
    MatSetValues(A,1,&row,3,cols,v,INSERT_VALUES);
  }
}
MatAssemblyBegin(A, MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A, MAT_FINAL_ASSEMBLY);
```

Advantages

All ranks busy: Scalable!

Amount of code essentially unchanged

Matrices

Definition (Matrix)

A matrix is a linear transformation between finite dimensional vector spaces.

Definition (Forming a matrix)

Forming or assembling a matrix means defining it's action in terms of entries (usually stored in a sparse format).

Important Matrices

1. Sparse (e.g. discretization of a PDE operator)
2. Inverse of *anything* interesting $B = A^{-1}$
3. Jacobian of a nonlinear function $Jy = \lim_{\epsilon \to 0} \frac{F(x+\epsilon y) - F(x)}{\epsilon}$
4. Fourier transform $\mathcal{F}, \mathcal{F}^{-1}$
5. Other fast transforms, e.g. Fast Multipole Method
6. Low rank correction $B = A + uv^T$
7. Schur complement $S = D - CA^{-1}B$
8. Tensor product $A = \sum_e A_x^e \otimes A_y^e \otimes A_z^e$
9. Linearization of a few steps of an explicit integrator

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9. Linearization of a few steps of an explicit integrator

These matrices are dense. Never form them.

Important Matrices

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These are not very sparse. Don't form them.

Important Matrices

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None of these matrices “have entries”

Iterative Solvers

Matrices

What can we do with a matrix that doesn't have entries?

Krylov solvers for $Ax = b$

Krylov subspace: $\{b, Ab, A^2b, A^3b, \dots\}$

Convergence rate depends on the spectral properties of the matrix

For any popular Krylov method $\mathcal{K}$, there is a matrix of size m, such that $\mathcal{K}$ outperforms all other methods by a factor at least $\mathcal{O}(\sqrt{m})$ [Nachtigal et. al., 1992]

Typically...

The action $y \leftarrow Ax$ can be computed in $\mathcal{O}(m)$

Aside from matrix multiply, the n^{th} iteration requires at most $\mathcal{O}(mn)$

GMRES

Brute force minimization of residual in $\{b, Ab, A^2b, \dots\}$

1. Use Arnoldi to orthogonalize the nth subspace, producing

$$AQ_n = Q_{n+1}H_n$$

2. Minimize residual in this space by solving the overdetermined system

$$H_n y_n = e_1^{(n+1)}$$

using QR-decomposition, updated cheaply at each iteration.

Properties

Converges in n steps for all right hand sides if there exists a polynomial of degree n such that $\|p_n(A)\| < \mathit{tol}$ and $p_n(0) = 1$.

Residual is monotonically decreasing, robust in practice

Restarted variants are used to bound memory requirements

Linear Solvers - Krylov Methods

Using PETSc linear algebra, just add:

```
KSPSetOperators(KSP ksp, Mat A, Mat M)
KSPSolve(KSP ksp, Vec b, Vec x)
```

Can access subobjects

```
KSPGetPC(KSP ksp, PC *pc)
```

Preconditioners must obey PETSc interface

- Basically just the KSP interface

Can change solver dynamically from the command line, `-ksp_type`

Linear solvers in PETSc KSP (Excerpt)

- Richardson
- Chebychev
- Conjugate Gradient
- BiConjugate Gradient
- Generalized Minimum Residual Variants
- Transpose-Free Quasi-Minimum Residual
- Least Squares Method
- Conjugate Residual

Preconditioners

Preconditioning

Idea: improve the conditioning of the Krylov operator

Left preconditioning

$$(P^{-1}A)x = P^{-1}b$$

$$\{P^{-1}b, (P^{-1}A)P^{-1}b, (P^{-1}A)^2P^{-1}b, \dots\}$$

Right preconditioning

$$(AP^{-1})Px = b$$

$$\{b, (P^{-1}A)b, (P^{-1}A)^2b, \dots\}$$

The product $P^{-1}A$ or AP^{-1} is *not* formed.

A *preconditioner* $\mathcal{P}$ is a method for constructing a matrix (just a linear function, not assembled!) $P^{-1} = \mathcal{P}(A, A_p)$ using a matrix A and extra information A_p, such that the spectrum of $P^{-1}A$ (or AP^{-1}) is well-behaved.

Preconditioning

Definition (Preconditioner)

A *preconditioner* $\mathcal{P}$ is a method for constructing a matrix $P^{-1} = \mathcal{P}(A, A_p)$ using a matrix A and extra information A_p, such that the spectrum of $P^{-1}A$ (or AP^{-1}) is well-behaved.

- P^{-1} is dense, P is often not available and is not needed
- A is rarely used by $\mathcal{P}$, but $A_p = A$ is common
- A_p is often a sparse matrix, the "preconditioning matrix"
- Matrix-based: Jacobi, Gauss-Seidel, SOR, ILU(k), LU
- Parallel: Block-Jacobi, Schwarz, Multigrid, FETI-DP, BDDC
- Indefinite: Schur-complement, Domain Decomposition, Multigrid

Questions to ask when you see a matrix

1. What do you want to do with it?
   - Multiply with a vector
   - Solve linear systems or eigen-problems
2. How is the conditioning/spectrum?
   - distinct/clustered eigen/singular values?
   - symmetric positive definite ($\sigma(A) \subset \mathbb{R}^+$)?
   - nonsymmetric definite ($\sigma(A) \subset \{z \in \mathbb{C} : \mathrm{Re}[z] > 0\}$)?
   - indefinite?
3. How dense is it?
   - block/banded diagonal?
   - sparse unstructured?
   - denser than we'd like?
4. Is there a better way to compute Ax?
5. Is there a different matrix with similar spectrum, but nicer properties?
6. How can we precondition A?

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Relaxation

Split into lower, diagonal, upper parts: $A = L + D + U$

Jacobi

Cheapest preconditioner: $P^{-1} = D^{-1}$

Relaxation

Split into lower, diagonal, upper parts: $A = L + D + U$

Jacobi

Cheapest preconditioner: $P^{-1} = D^{-1}$

Successive over-relaxation (SOR)

$$\left(L + \frac{1}{\omega}D\right) x_{n+1} = \left[\left(\frac{1}{\omega} - 1\right) D - U\right] x_n + \omega b$$

$P^{-1} = k$ iterations starting with $x_0 = 0$

Implemented as a sweep

$\omega = 1$ corresponds to Gauss-Seidel

Very effective at removing high-frequency components of residual

Factorization

Two phases

symbolic factorization: find where fill occurs, only uses sparsity pattern
numeric factorization: compute factors

Factorization

Two phases

symbolic factorization: find where fill occurs, only uses sparsity pattern
numeric factorization: compute factors

LU decomposition

Ultimate preconditioner
Expensive, for $m \times m$ sparse matrix with bandwidth b, traditionally requires $\mathcal{O}(mb^2)$ time and $\mathcal{O}(mb)$ space.

- Bandwidth scales as $m^{\frac{d-1}{d}}$ in d-dimensions
- Optimal in 2D: $\mathcal{O}(m \cdot \log m)$ space, $\mathcal{O}(m^{3/2})$ time
- Optimal in 3D: $\mathcal{O}(m^{4/3})$ space, $\mathcal{O}(m^2)$ time

Symbolic factorization is problematic in parallel

Factorization

Two phases

symbolic factorization: find where fill occurs, only uses sparsity pattern
numeric factorization: compute factors

LU decomposition

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Symbolic factorization is problematic in parallel

Incomplete LU

Allow a limited number of levels of fill: ILU(k)
Only allow fill for entries that exceed threshold: ILUT
Usually poor scaling in parallel
No guarantees

1-level Domain decomposition

Domain size L, subdomain size H, element size h

Overlapping/Schwarz

Solve Dirichlet problems on overlapping subdomains

No overlap: *its* $\in \mathcal{O}\left(\frac{L}{\sqrt{Hh}}\right)$

Overlap δ: *its* $\in \left(\frac{L}{\sqrt{H\delta}}\right)$

1-level Domain decomposition

Domain size L, subdomain size H, element size h

Overlapping/Schwarz

Solve Dirichlet problems on overlapping subdomains

No overlap: *its* $\in \mathcal{O}\left(\frac{L}{\sqrt{Hh}}\right)$

Overlap δ: *its* $\in \left(\frac{L}{\sqrt{H\delta}}\right)$

Neumann-Neumann

Solve Neumann problems on non-overlapping subdomains

its $\in \mathcal{O}\left(\frac{L}{H}(1+\log\frac{H}{h})\right)$

Tricky null space issues (floating subdomains)

Need subdomain matrices, net globally assembled matrix.

Multilevel variants knock off the leading $\frac{L}{H}$

Both overlapping and nonoverlapping with this bound

Multigrid

Hierarchy: Interpolation and restriction operators

$$\mathcal{I}^{\uparrow} : X_{\text{coarse}} \to X_{\text{fine}} \qquad \mathcal{I}^{\downarrow} : X_{\text{fine}} \to X_{\text{coarse}}$$

Geometric: define problem on multiple levels, use grid to compute hierarchy
Algebraic: define problem only on finest level, use matrix structure to build hierarchy

Galerkin approximation

Assemble this matrix: $A_{\text{coarse}} = \mathcal{I}^{\downarrow} A_{\text{fine}} \mathcal{I}^{\uparrow}$

Application of multigrid preconditioner (V-cycle)

Apply pre-smoother on fine level (any preconditioner)
Restrict residual to coarse level with $\mathcal{I}^{\downarrow}$
Solve on coarse level $A_{\text{coarse}} x = r$
Interpolate result back to fine level with $\mathcal{I}^{\uparrow}$
Apply post-smoother on fine level (any preconditioner)

Multigrid convergence properties

Textbook: $P^{-1}A$ is spectrally equivalent to identity
- Constant number of iterations to converge up to discretization error

Most theory applies to SPD systems
- variable coefficients (e.g. discontinuous): low energy interpolants
- mesh- and/or physics-induced anisotropy: semi-coarsening/line smoothers
- complex geometry: difficult to have meaningful coarse levels

Deeper algorithmic difficulties
- nonsymmetric (e.g. advection, shallow water, Euler)
- indefinite (e.g. incompressible flow, Helmholtz)

Performance considerations
- Aggressive coarsening is critical in parallel
- Most theory uses SOR smoothers, ILU often more robust
- Coarsest level usually solved semi-redundantly with direct solver

Multilevel Schwarz is essentially the same with different language
- assume strong smoothers, emphasize aggressive coarsening

Splitting for Multiphysics

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

Relaxation: `-pc_fieldsplit_type [additive,multiplicative,symmetric_multiplicative]`

$$\begin{bmatrix} A & \\ & D \end{bmatrix}^{-1} \qquad \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \qquad \begin{bmatrix} A & \\ & \mathbf{1} \end{bmatrix}^{-1} \left(\mathbf{1} - \begin{bmatrix} A & B \\ & \mathbf{1} \end{bmatrix} \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \right)$$

Gauss-Seidel inspired, works when fields are loosely coupled

Factorization: `-pc_fieldsplit_type schur`

$$\begin{bmatrix} A & B \\ & S \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{1} & \\ CA^{-1} & \mathbf{1} \end{bmatrix}^{-1}, \qquad S = D - CA^{-1}B$$

robust (exact factorization), can often drop lower block
how to precondition S which is usually dense?

interpret as differential operators, use approximate commutators

Distributed Arrays

Distributed Array

Interface for topologically structured grids

Defines (topological part of) a finite-dimensional function space

Get an element from this space: `DMCreateGlobalVector()`

Provides parallel layout

Refinement and coarsening

`DMRefineHierarchy()`

Ghost value coherence

`DMGlobalToLocalBegin()`

Matrix preallocation

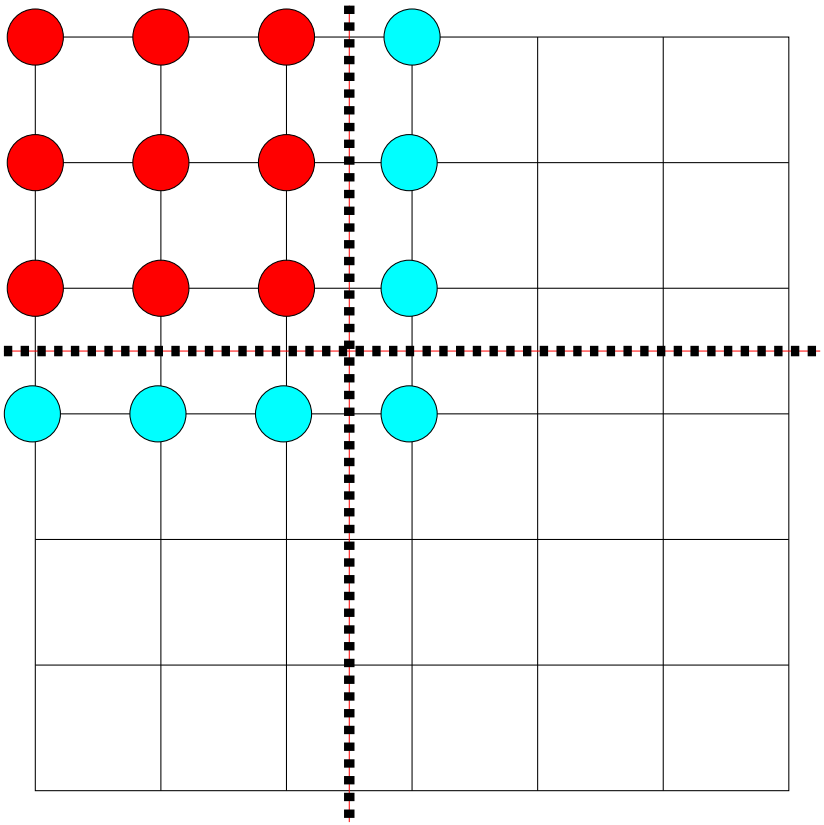
`DMCreateMatrix()` (formerly `DMGetMatrix()`)

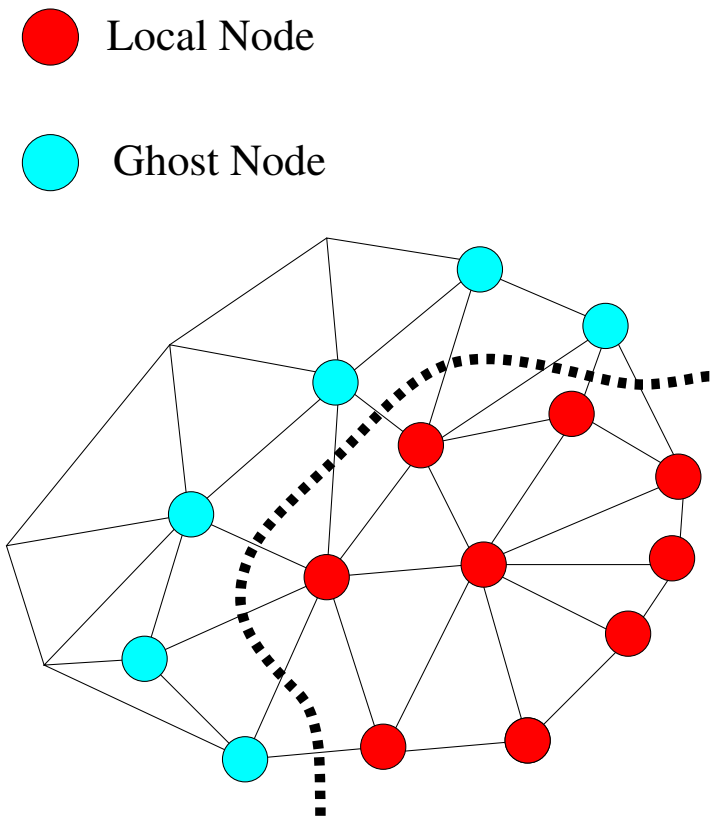
Ghost Values

To evaluate a local function $f(x)$, each process requires

its local portion of the vector x

its ghost values, bordering portions of x owned by neighboring processes





DMDA Global Numberings

Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
15	16	17	18	19
10	11	12	13	14
5	6	7	8	9
0	1	2	3	4
Proc 0			Proc 1	

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

PETSc numbering

DMDA Global vs. Local Numbering

Global: Each vertex has a unique id, belongs on a unique process

Local: Numbering includes vertices from neighboring processes

These are called ghost vertices

Proc 2			Proc 3	
X	X	X	X	X
X	X	X	X	X
12	13	14	15	X
8	9	10	11	X
4	5	6	7	X
0	1	2	3	X
Proc 0			Proc 1	

Local numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
3	4	5	11	12
0	1	2	9	10
Proc 0			Proc 1	

Global numbering

DM Vectors

The DM object contains only layout (topology) information

All field data is contained in PETSc `Vec`s

Global vectors are parallel

Each process stores a unique local portion

```
DMCreateGlobalVector(DM dm, Vec *gvec)
```

Local vectors are sequential (and usually temporary)

Each process stores its local portion plus ghost values

```
DMCreateLocalVector(DM dm, Vec *lvec)
```

includes ghost values!

Coordinate vectors store the mesh geometry

```
DMDAGetCoordinates(DM dm, Vec *coords)
```

Can be manipulated with their own DMDA

```
DMDAGetCoordinateDA(DM dm,DM *cda)
```

Updating Ghosts

Two-step Process for Updating Ghosts

enables overlapping computation and communication

`DMGlobalToLocalBegin(dm, gvec, mode, lvec)`

`gvec` provides the data

`mode` is either `INSERT_VALUES` or `ADD_VALUES`

`lvec` holds the local and ghost values

`DMGlobalToLocalEnd(dm, gvec, mode, lvec)`

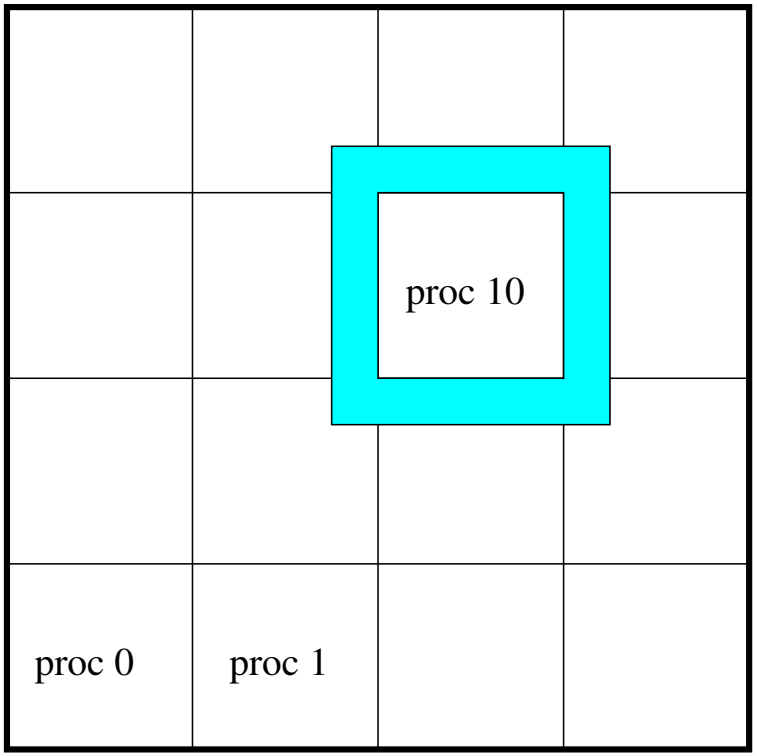
Finishes the communication

Reverse Process

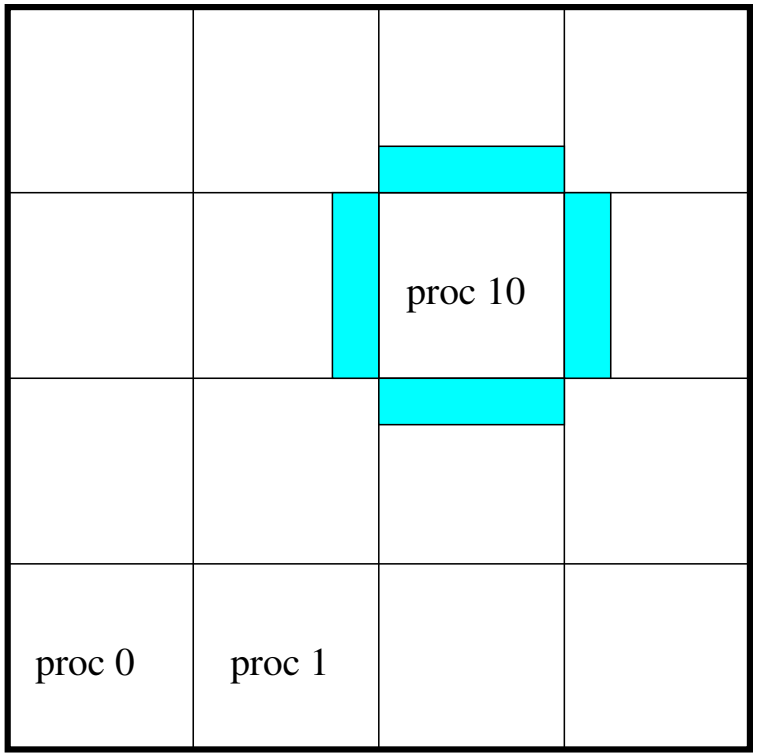
Via `DMLocalToGlobalBegin()` and `DMLocalToGlobalEnd()`.

DMDA Stencils

Available Stencils



Box Stencil



Star Stencil

Creating a DMDA

```
DMDACreate2d(comm, xbdy, ybdy, type, M, N, m, n,
             dof, s, lm[], ln[], DA *da)
```

`xbdy,ybdy`: Specifies periodicity or ghost cells

`DM_BOUNDARY_NONE`, `DM_BOUNDARY_GHOSTED`, `DM_BOUNDARY_MIRROR`, `DM_BOUNDARY_PERIODIC`

`type`

Specifies stencil: `DMDA_STENCIL_BOX` or `DMDA_STENCIL_STAR`

`M,N`

Number of grid points in x/y-direction

`m,n`

Number of processes in x/y-direction

`dof`

Degrees of freedom per node

`s`

The stencil width

`lm,ln`

Alternative array of local sizes

Use `NULL` for the default

Working with the Local Form

Wouldn't it be nice if we could just write our code for the natural numbering?

Proc 2			Proc 3	
25	26	27	28	29
20	21	22	23	24
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Proc 0			Proc 1	

Natural numbering

Proc 2			Proc 3	
21	22	23	28	29
18	19	20	26	27
15	16	17	24	25
6	7	8	13	14
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0	1	2	9	10
Proc 0			Proc 1	

PETSc numbering

Working with the Local Form

Wouldn't it be nice if we could just write our code for the natural numbering?

Yes, that's what `DMDAVecGetArray()` is for.

DMDA offers *local* callback functions

`FormFunctionLocal()`, set by `DMDASetLocalFunction()`

`FormJacobianLocal()`, set by `DMDASetLocalJacobian()`

Evaluating the nonlinear residual $F(x)$

Each process evaluates the local residual

PETSc assembles the global residual automatically

Uses `DMLocalToGlobal()` method

Thinking of Extensions

Multiple Unknowns per Grid Node

Example 1: Displacements u_x, u_y

Example 2: Velocity components, Pressure

Typical in a multiphysics setting

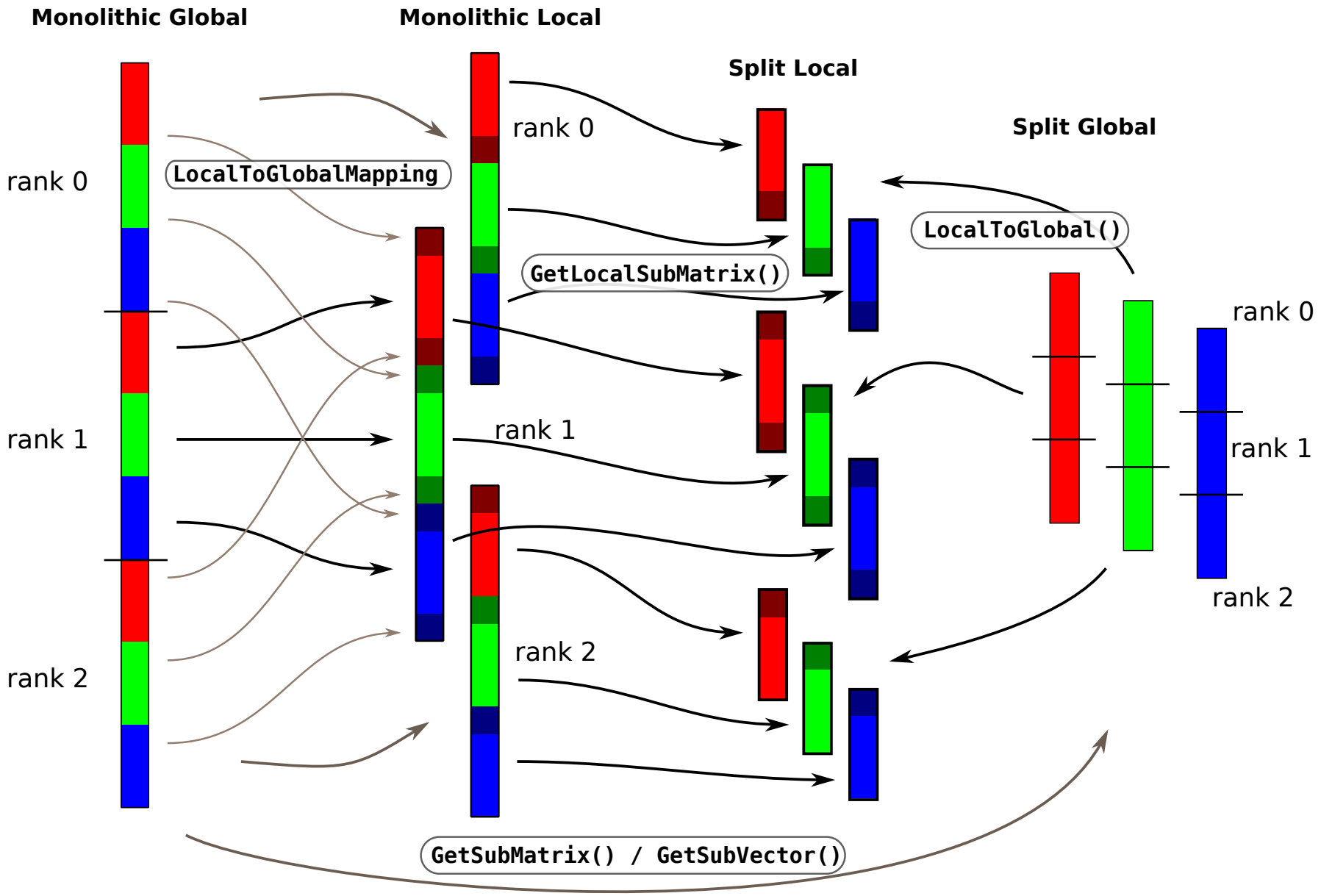
Multiple Unknowns in a Distributed Setting

Robust abstract concepts important

Lots of bookkeeping

All done by PETSc

Thinking of Extensions



DA Local Function

User-provided Function for Nonlinear Residual in 2D

```
PetscErrorCode (*lfunc)(DMDALocalInfo *info,
                        Field **x, Field **r,
                        void *ctx)
```

`info`	All layout and numbering information
`x`	The current solution *Notice that it is a multidimensional array*
`r`	The residual
`ctx`	The user context passed to `DMSetApplicationContext()` or to SNES

The local DMDA function is activated by calling

```
SNESSetDM(snes,dm)
SNESSetFunction(snes, r, SNESDAFormFunction, ctx)
```

End of Morning Session

PETSc Can Help You

solve algebraic and DAE problems in your application area

rapidly develop efficient parallel code, can start from examples

develop new solution methods and data structures

debug and analyze performance

advice on software design, solution algorithms, and performance

`petsc-{users,dev,maint}@mcs.anl.gov`

You Can Help PETSc

report bugs and inconsistencies, or if you think there is a better way

tell us if the documentation is inconsistent or unclear

consider developing new algebraic methods as plugins, contribute if your idea works