Using PETSc for scientific computing in parallel

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This talk comes out of joint work on PISM with
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Thanks to Don Bahls *at ARSC for help making it all work on the big machines.*

Outline

Outline

PETSc = Portable Extensible Toolkit for Scientific computation

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.

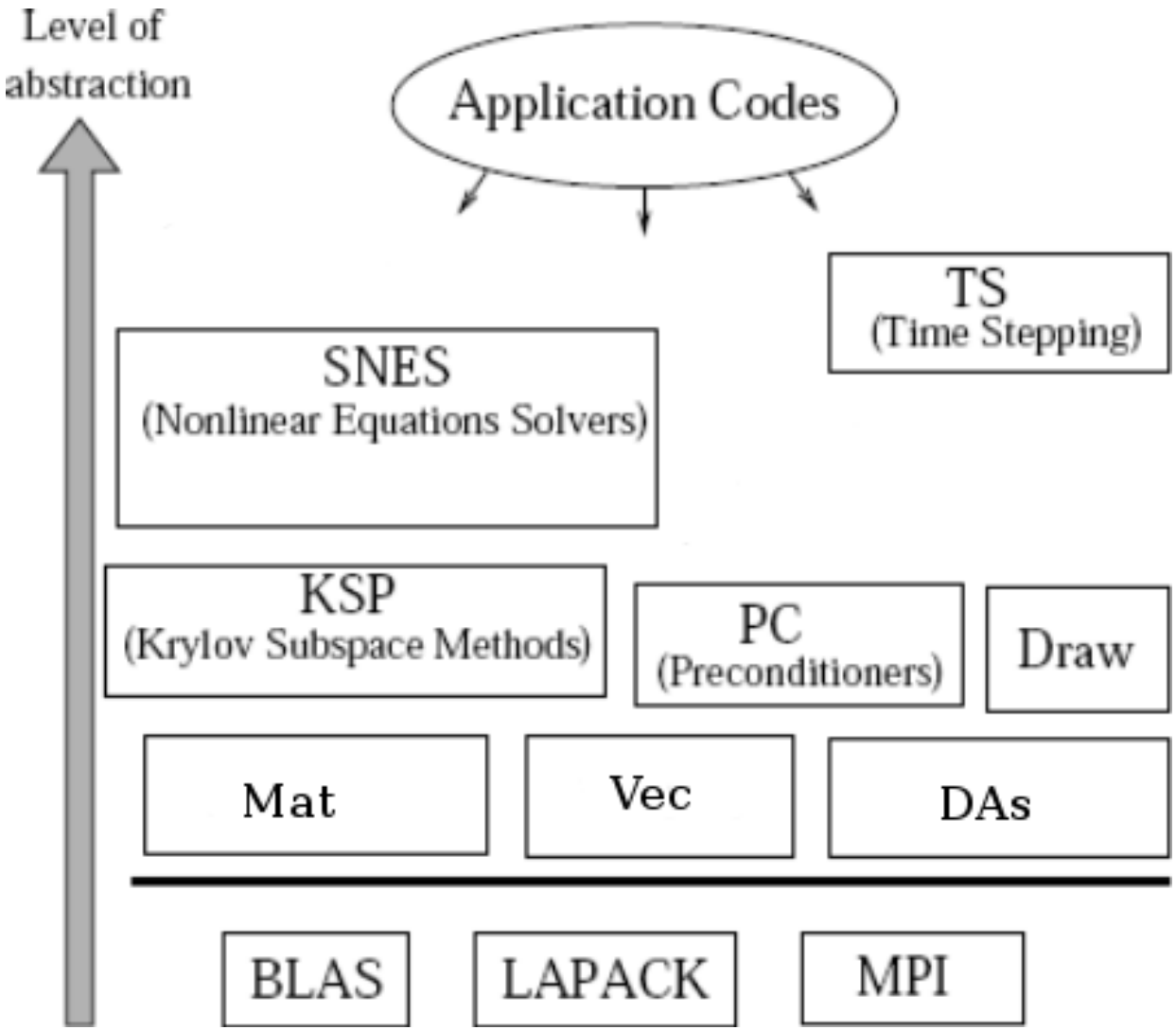
–Barry Smith, a PETSc developer since its start in 1991

PETSc

"PETSc Overview" section MOSTLY STOLEN FROM TUTORIAL SLIDES BY Matt Knepley:
http://www-unix.mcs.anl.gov/petsc/petsc-2/documentation/tutorials/PCFD2007.pdf

- download from `http://www.mcs.anl.gov/petsc` at Argonne National Lab (the MPI people)
- free for everyone, including industrial users
- hyperlinked manual, examples, and manual pages; hundreds of tutorial-style examples
- written in C but used from C, C++, Fortran 77/90, and Python; lots of Fortran users
- PETSc has run problems with over 500 million unknowns
- PETSc has run on over 6,000 processors efficiently
- PETSc applications have run at 2 Teraflops: LANL PFLOTRAN code

PETSc as a level of abstraction



PETSc uses MPI

- the Message Passing Interface is:
  - a library for parallel communication
  - a launcher for parallel jobs (`mpiexec`)
  - a community standard
- creators of MPI imagined most users would work at higher level of abstraction, *like the level in* PETSc
- you should *almost* never have to make MPI calls when using PETSc
- PETSc uses two default MPI communicators, yourself (`PETSC_COMM_SELF`) and everyone launched (`PETSC_COMM_WORLD`)
- PETSc uses MPI for point-to-point communication (like in `MatMult()`) and for reduction or scan operations among all processes (like in `VecDot()`)

extensions of PETSc

- libMesh, DEALII, Prometheus for meshing and finite element solns of PDEs
- TAO for optimization
- SLEPc for eigenvalue problems

configure and build PETSc: brief version

- set `PETSC_DIR` to the installation root directory
- run the configuration utility `$PETSC_DIR/config/configure.py`
  - there are many examples on the installation page
  - configuration files are placed in `$PETSC_DIR/bmake/$PETSC_ARCH`
  - `$PETSC_ARCH` has a default if not specified
- `make all test`
- try running PETSc examples first:
  - `cd $PETSC_DIR/src/snes/examples/tutorials`
  - `make ex5`
  - `./ex5`
  - `mpiexec -np 4 ./ex5`

Caveat about this talk

- PETSc is big. It is many things to many people.
- I will talk about the parts of PETSc I have used the most:
  - structured grids for finite differences and
  - linear algebra (as a part of the solution of nonlinear PDEs.)

Outline

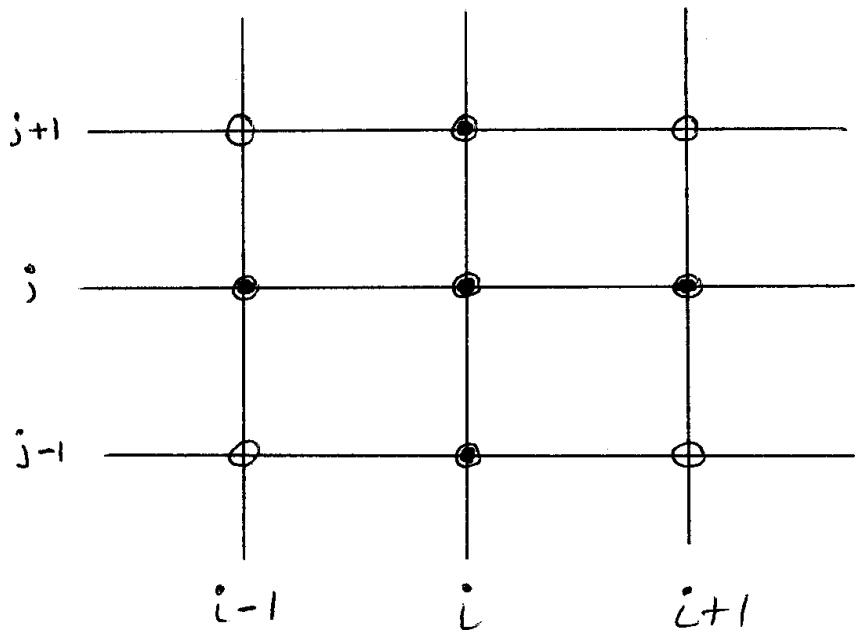
DA = Distributed Array

the DA abstract data type:

- is a structured grid interface
- is for fixed simple topologies
- supports stencils, communication, reordering
- is nice for simple finite differences

at right:

- circles are BOX stencil
- solid dots are STAR stencil

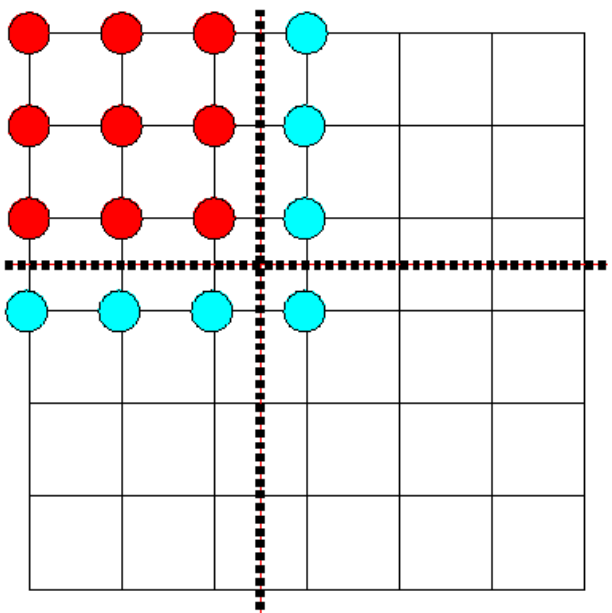


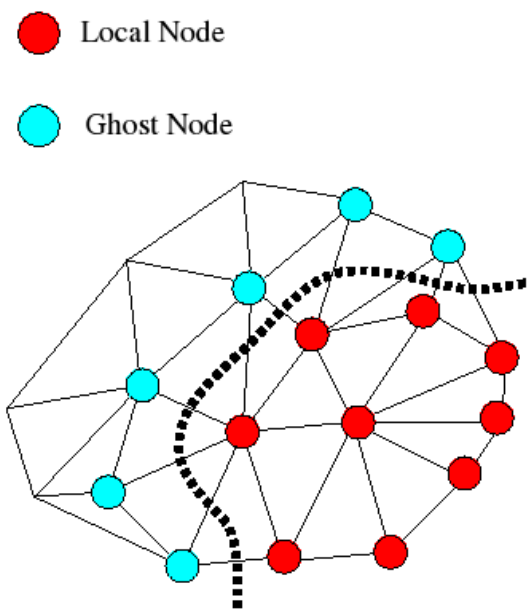
(there are also PETSc Mesh and DMMG abstract data types for finite elements and multigrid, resp.)

Ghosted points

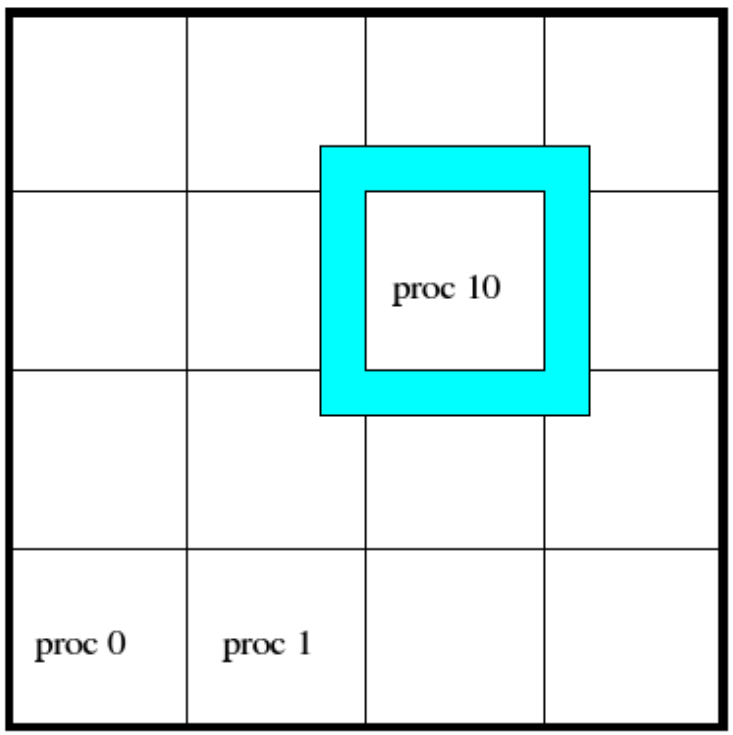
Why use DA abstraction?

- much parallel scientific computing is on a grid and has stereotyped communication
- one grid point needs to communicate with its neighbors at each time step, but not with distant grid points
- DAs manage this communication in *rectangular grid case* (left)
- no direct MPI calls to communicate values at neighbors on different processors

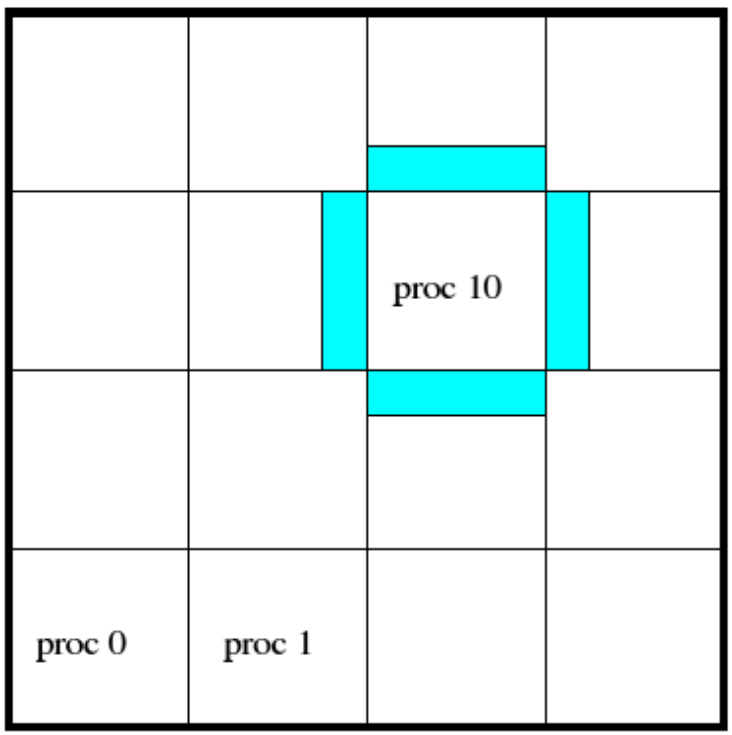




Inter-process communication for BOX versus STAR



Box Stencil



Star Stencil

Creating a 2d DA

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

wrap: Specifies periodicity
- DA_NONPERIODIC, DA_XPERIODIC, DA_YPERIODIC, or DA_XYPERIODIC

type: Specifies stencil
- DA_STENCIL_BOX or DA_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/n: Alternative array of local sizes
- Use PETSC_NULL for the default

Creating a 3d DA

same, but with another dimension

DA manages a Vec

create DA, then creates Vecs managed by it; "local" Vecs carry their ghosted points while "global" Vecs do not; for example:

```
DA  da;
Vec v;

DACreate2d(com, DA_XYPERIODIC, DA_STENCIL_BOX,
    M, N, PETSC_DECIDE, PETSC_DECIDE,
    1, 1, PETSC_NULL, PETSC_NULL, &da);
DACreateLocalVector(da, &v);
for (k=0; k<steps; k++) { // e.g. time stepping loop
   [  MANIPULATIONS USING VALUES AT GHOSTED POINTS ]
   [  AND MODIFYING VALUES AT NON-GHOSTED POINTS        ]
   // now communicate and update ghosted points
   DALocalToLocalBegin(da, v, INSERT_VALUES, v);
   DALocalToLocalEnd(da, v, INSERT_VALUES, v);
}
VecDestroy(v);
DADestroy(da);
```

Outline

a program that does nothing, but in parallel!

nothin.c:

```
static char help[] = "A string for -help.\n";
#include <petscvec.h>
int main(int argc, char *argv[]) {
  PetscErrorCode  ierr;
  PetscMPIInt rank, size;

  ierr = PetscInitialize(&argc, &argv, PETSC_NULL, help); CHKERRQ(ierr);
  ierr = MPI_Comm_rank(PETSC_COMM_WORLD, &rank); CHKERRQ(ierr);
  ierr = MPI_Comm_size(PETSC_COMM_WORLD, &size); CHKERRQ(ierr);

  ierr = PetscPrintf(PETSC_COMM_SELF,"rank = %d\n",rank);CHKERRQ(ierr);
  ierr = PetscPrintf(PETSC_COMM_WORLD,"size = %d\n",size);CHKERRQ(ierr);

  ierr = PetscFinalize(); CHKERRQ(ierr);
  return 0;
}
```

make a PETSc application

makefile:

```
include ${PETSC_DIR}/bmake/common/base

nothin: nothin.o  chkopts
    -${CLINKER} -o nothin nothin.o ${PETSC_LIB}
```

run a PETSc application

```
$ make nothin
...
$ ./nothin
rank = 0
size = 1
$ mpiexec -n 4 ./nothin
rank = 0
size = 4
rank = 2
rank = 3
rank = 1
```

setting up a DA and a Vec

davec.c:

```
#include <petscda.h>

int main(int argc, char *argv[]) {
  PetscErrorCode  ierr;
  PetscMPIInt     rank;
  PetscInt        myM = 50, myN = 53;
  DA              da2;
  DALocalInfo     info;
  Vec             vv;

  PetscInitialize(&argc, &argv, PETSC_NULL, help);
  MPI_Comm_rank(PETSC_COMM_WORLD, &rank);
  PetscOptionsGetInt(PETSC_NULL, "-M", &myM, PETSC_NULL);
  PetscOptionsGetInt(PETSC_NULL, "-N", &myN, PETSC_NULL);
```

setting up a DA and a Vec

davec.c cont.:

```
  DACreate2d(PETSC_COMM_WORLD, DA_XYPERIODIC, DA_STENCIL_STAR,
             myM, myN, PETSC_DECIDE, PETSC_DECIDE,
             1, 1, PETSC_NULL, PETSC_NULL, &da2);
  DAGetLocalInfo(da2, &info); CHKERRQ(ierr);
  PetscPrintf(PETSC_COMM_WORLD,
           "  whole grid size is %d x %d\n",myM,myN); CHKERRQ(ierr);
  PetscPrintf(PETSC_COMM_SELF,
           "  grid ranges for rank %d process:  xs=%d, xm=%d, ys=%d, ym=%d\n",
           rank,info.xs,info.xm,info.ys,info.ym);
  DACreateGlobalVector(da2, &vv);

  // could do something with vv here

  VecDestroy(vv);
  DADestroy(da2);
  PetscFinalize();
  return 0;
}
```

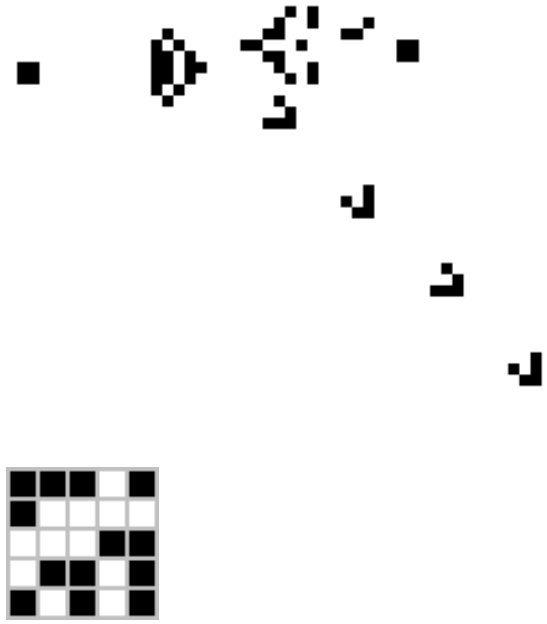
setting up a DA and a Vec

```
$ ./davec -M 200 -N 200
  whole grid size is 200 x 200
  grid ranges for rank 0 process:  xs=0, xm=200, ys=0, ym=200
$ mpiexec -n 6 ./davec -M 200 -N 200
  grid ranges for rank 1 process:  xs=100, xm=100, ys=0, ym=67
  grid ranges for rank 4 process:  xs=0, xm=100, ys=134, ym=66
  grid ranges for rank 5 process:  xs=100, xm=100, ys=134, ym=66
  whole grid size is 200 x 200
  grid ranges for rank 0 process:  xs=0, xm=100, ys=0, ym=67
  grid ranges for rank 2 process:  xs=0, xm=100, ys=67, ym=67
  grid ranges for rank 3 process:  xs=100, xm=100, ys=67, ym=67
```

John Conway's "Life" in parallel

Goal: Write a PETSc program using a `BOX` stencil `DA` for Life.

```
double lifeRule(double me, double nsum) {
   if (fabs(me - 0.0) < 0.1) { // dead cell
     if (fabs(nsum - 3.0) < 0.1)  return 1.0;
     else  return 0.0;
   } else { // live cell
     if (nsum < 1.9)  return 0.0;
     else if (nsum > 3.1)  return 0.0;
     else  return 1.0;
   }
}
```



"Life" in parallel

life.c:

```
int main(int argc, char *argv[]) {
  ...
  PetscScalar     startPattern[5][5] = {1.0, 1.0, 1.0, 0.0, 1.0,
                                       1.0, 0.0, 0.0, 0.0, 0.0,
                                       0.0, 0.0, 0.0, 1.0, 1.0,
                                       0.0, 1.0, 1.0, 0.0, 1.0,
                                       1.0, 0.0, 1.0, 0.0, 1.0};

  // start up and read options ...
  ierr = DACreate2d(PETSC_COMM_WORLD, DA_XYPERIODIC, DA_STENCIL_BOX,
            myM, myN, PETSC_DECIDE, PETSC_DECIDE, 1, 1, PETSC_NULL,
            PETSC_NULL, &da2); CHKERRQ(ierr);
  ierr = DAGetLocalInfo(da2, &info); CHKERRQ(ierr);
  ierr = DACreateGlobalVector(da2, &gstate); CHKERRQ(ierr);
  // set initial state ...
  // set ghosted values on each processor
  ierr = DACreateLocalVector(da2, &lstate); CHKERRQ(ierr);
  ierr = DAGlobalToLocalBegin(da2, gstate, INSERT_VALUES, lstate);
  ierr = DAGlobalToLocalEnd(da2, gstate, INSERT_VALUES, lstate);
  // view initial state ...
```

"Life" in parallel

life.c cont.:

```
  for (k = 0; k < max_steps; k++) {
    ierr = DAVecGetArray(da2, gstate, &st); CHKERRQ(ierr);
    ierr = DAVecGetArray(da2, lstate, &ost); CHKERRQ(ierr);
    for (i=info.xs; i<info.xs+info.xm; ++i) {
      for (j=info.ys; j<info.ys+info.ym; ++j) {
        nsum = ost[j][i+1] + ost[j-1][i+1] + ost[j-1][i] + ost[j-1][i-1] +
               ost[j][i-1] + ost[j+1][i-1] + ost[j+1][i] + ost[j+1][i+1]);
        st[j][i] = lifeRule(ost[j][i],nsum)
      }
    }
    ierr = DAVecRestoreArray(da2, lstate, &ost); CHKERRQ(ierr);
    ierr = DAVecRestoreArray(da2, gstate, &st); CHKERRQ(ierr);
    // update ghosted values from new (global) state on each processor
    ierr = DAGlobalToLocalBegin(da2, gstate, INSERT_VALUES, lstate);
    ierr = DAGlobalToLocalEnd(da2, gstate, INSERT_VALUES, lstate);
    ierr = VecView(gstate, viewer); CHKERRQ(ierr);
  }
  // finish up ...
}
```

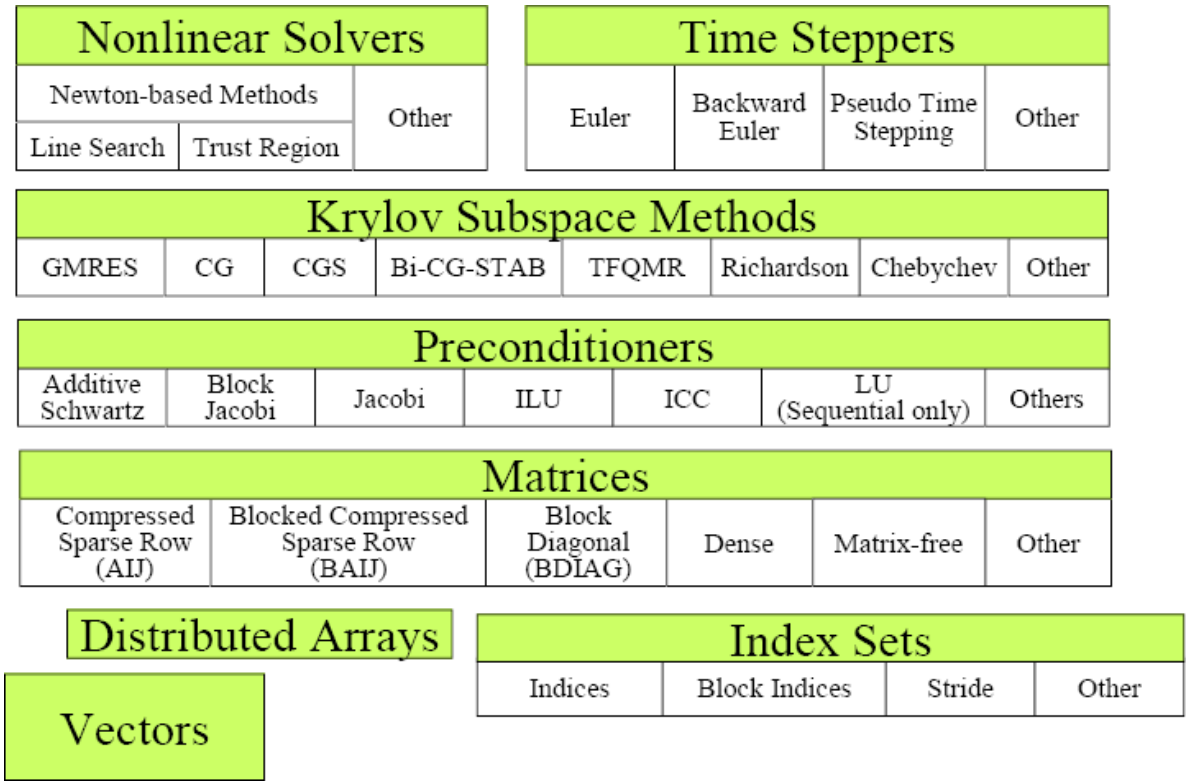
"Life" in parallel

```
$   make life

$   ./life

$   mpiexec -n 4 ./life -display :0
```

ED: RUN IT

Outline

Mathematical tools in PETSc



next in *this* talk

- matrices (`Mat` type)
- Krylov methods (`KSP` type)
- preconditioners

Linear algebra in parallel: Ideas

To solve $A\mathbf{x} = \mathbf{b}$:

- big problems frequently have sparse A
- so store A sparsely
- LU decomposition usually bad because fill-in
- Krylov subspace idea:
  - soln to $A\mathbf{x} = \mathbf{b}$ frequently well-approximated by element of subspace spanned by $\{\mathbf{b}, A\mathbf{b}, A^2\mathbf{b}, \ldots, A^k\mathbf{b}\}$
  - so $\mathbf{x}$ well approximated by $p(A)\mathbf{b}$ where p is a polynomial
  - spectrum of A critical to ease of polynomial approximation
- precondition to get spectum in better position:
  $A\mathbf{x} = \mathbf{b} \quad \longrightarrow MA\mathbf{x} = M\mathbf{b}$
- PETSc *implements all these ideas* and *allows control of it at runtime*; examples next

Example of matrices and KSP

next few slides use `$PETSC_DIR/src/ksp/ksp/examples/tutorials/ex2.c`, an example code included in PETSc distribution, to illustrate `Mat` and `KSP` uses

- even on a regular grid, sometimes one needs to solve a set of equations
- values at distant grid points couple together through many equations

For example, finite difference approximation of Poisson eqn:

$$u_{xx} + u_{yy} = f$$

$$\downarrow$$

$$U_{i+1,j} + U_{i-1,j} + U_{i,j+1} + U_{i,j-1} - 4U_{i,j} = (\text{known})$$

next: `ex2.c` sets up and solves this problem

Mat and KSP example

ex2.c:

```
#include "petscksp.h"

int main(int argc,char **args)
{
  Vec            x,b,u;  /* approx solution, RHS, exact solution */
  Mat            A;        /* linear system matrix */
  KSP            ksp;     /* linear solver context */
  PetscReal      norm;     /* norm of solution error */
  PetscInt       i,j,Ii,J,Istart,Iend,m = 8,n = 7,its;

  [ deleted: INITIALIZE AND GET OPTIONS ]
  MatCreate(PETSC_COMM_WORLD,&A);
  MatSetSizes(A,PETSC_DECIDE,PETSC_DECIDE,m*n,m*n);
  MatSetType(A, MATAIJ);
  MatSetFromOptions(A);
  MatMPIAIJSetPreallocation(A,5,PETSC_NULL,5,PETSC_NULL);
  MatSeqAIJSetPreallocation(A,5,PETSC_NULL);
  MatGetOwnershipRange(A,&Istart,&Iend);
```

Mat and KSP example

ex2.c cont.:

```
for (Ii=Istart; Ii<Iend; Ii++) {
  v = -1.0; i = Ii/n; j = Ii - i*n;
  if (i>0)   {J = Ii - n; MatSetValues(A,1,&Ii,1,&J,&v,INSERT_VALUES);}
  if (i<m-1) {J = Ii + n; MatSetValues(A,1,&Ii,1,&J,&v,INSERT_VALUES);}
  if (j>0)   {J = Ii - 1; MatSetValues(A,1,&Ii,1,&J,&v,INSERT_VALUES);}
  if (j<n-1) {J = Ii + 1; MatSetValues(A,1,&Ii,1,&J,&v,INSERT_VALUES);}
  v = 4.0; ierr = MatSetValues(A,1,&Ii,1,&Ii,&v,INSERT_VALUES);
}
MatAssemblyBegin(A,MAT_FINAL_ASSEMBLY);
MatAssemblyEnd(A,MAT_FINAL_ASSEMBLY);
VecCreate(PETSC_COMM_WORLD,&u);
VecSetSizes(u,PETSC_DECIDE,m*n);
VecSetFromOptions(u);
VecDuplicate(u,&b);
VecDuplicate(b,&x);
[ deleted: SET EXACT SOLUTION FOR COMPARISON ]
```

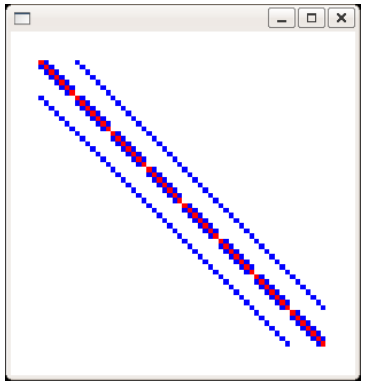
Mat and KSP example

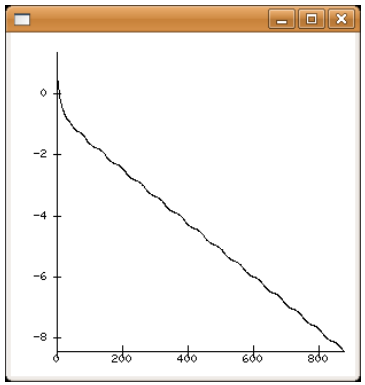
ex2.c cont. cont.:

```
  KSPCreate(PETSC_COMM_WORLD,&ksp);
  KSPSetOperators(ksp,A,A,DIFFERENT_NONZERO_PATTERN);
  KSPSetTolerances(ksp,1.e-2/((m+1)*(n+1)),1.e-50,PETSC_DEFAULT,
                   PETSC_DEFAULT);
  KSPSetFromOptions(ksp);
  KSPSolve(ksp,b,x);
  [ deleted: COMPARE TO EXACT SOLUTION ]
  PetscPrintf(PETSC_COMM_WORLD,"Norm of error %A iterations %D\n",
              norm,its);
  KSPDestroy(ksp);
  VecDestroy(u);   VecDestroy(x);
  VecDestroy(b);   MatDestroy(A);
  PetscFinalize();
  return 0;
}
```

Controlling tolerance and method

PETSc allows control at command line of method and accuracy; also viewing of internal `Vec`, `Mat`, and `KSP` objects:






```
$  ./ex2
Norm of error 0.000156044 iterations 6
$  mpiexec -n 6 ./ex2
Norm of error 0.000709535 iterations 11
$ ./ex2 -ksp_type cgs
Norm of error 7.69507e-05 iterations 4
$ ./ex2 -ksp_rtol 1e-10
Norm of error 1.49481e-10 iterations 13
$ mpiexec -n 6 ./ex2 -m 200 -n 200
Norm of error 0.0051396 iterations 404
$ mpiexec -n 6 ./ex2 -m 200 -n 200 -pc_type asm
Norm of error 0.0041435 iterations 359
$ ./ex2 -mat_view_draw
Norm of error 0.000156044 iterations 6
$ ./ex2 -ksp_monitor_draw -ksp_rtol 1e-12 -m 300 -n 300
Norm of error 5.65271e-08 iterations 1127
```

Does result depend on number of processors?

Can a PETSc linear algebra result depend on number of processors?

- *yes*, sometimes
- the KSP act the same on different numbers of processors
- the *preconditioner* acts differently
- one may *turn off the preconditioner* to get independence of number of processors; generally slower convergence without preconditioner

```
$  mpiexec -n 1 ./ex2
Norm of error 0.000156044 iterations 6
$  mpiexec -n 6 ./ex2
Norm of error 0.000709535 iterations 11
$  mpiexec -n 1 ./ex2 -pc_type none
Norm of error 1.68964e-05 iterations 13
$  mpiexec -n 6 ./ex2 -pc_type none
Norm of error 1.68964e-05 iterations 13
```

No conclusion. Just back to work . . .

- talk to me about PETSc anytime, or email the maintainers, *who do check their email*!
- codes `nothin.c`, `davec.c`, `life.c`, `ex2.c` all available [HOW?]
- many problems don't need PETSc, as *Matlab* will do them just fine
- numerical algorithm improvements usually more effective than parallelization

Thanks for your attention or tolerance!