Introduction to PETSc

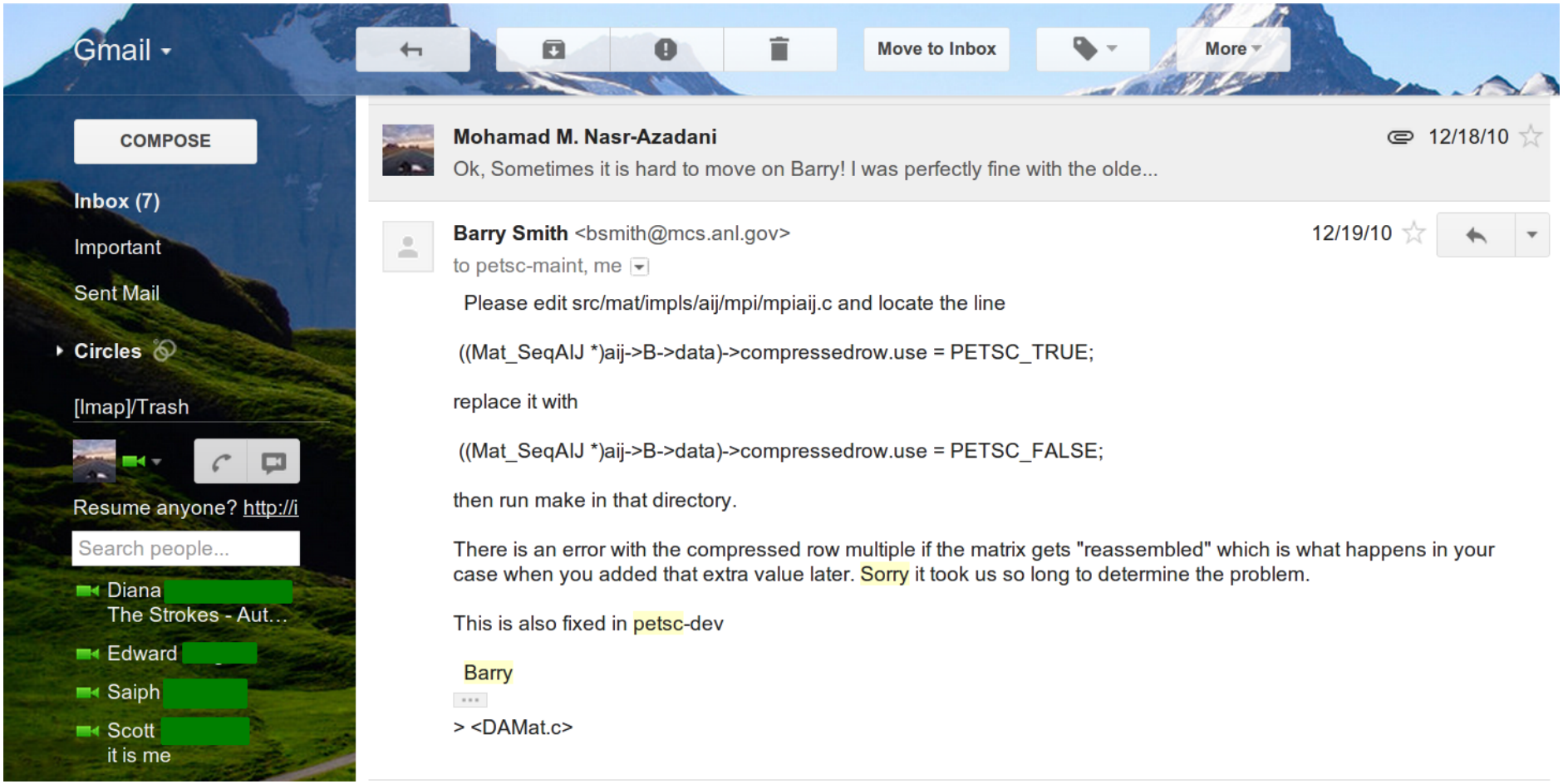
Mohamad M. Nasr-Azadani

Mechanical Engineering Department,
University of California at Santa Barbara

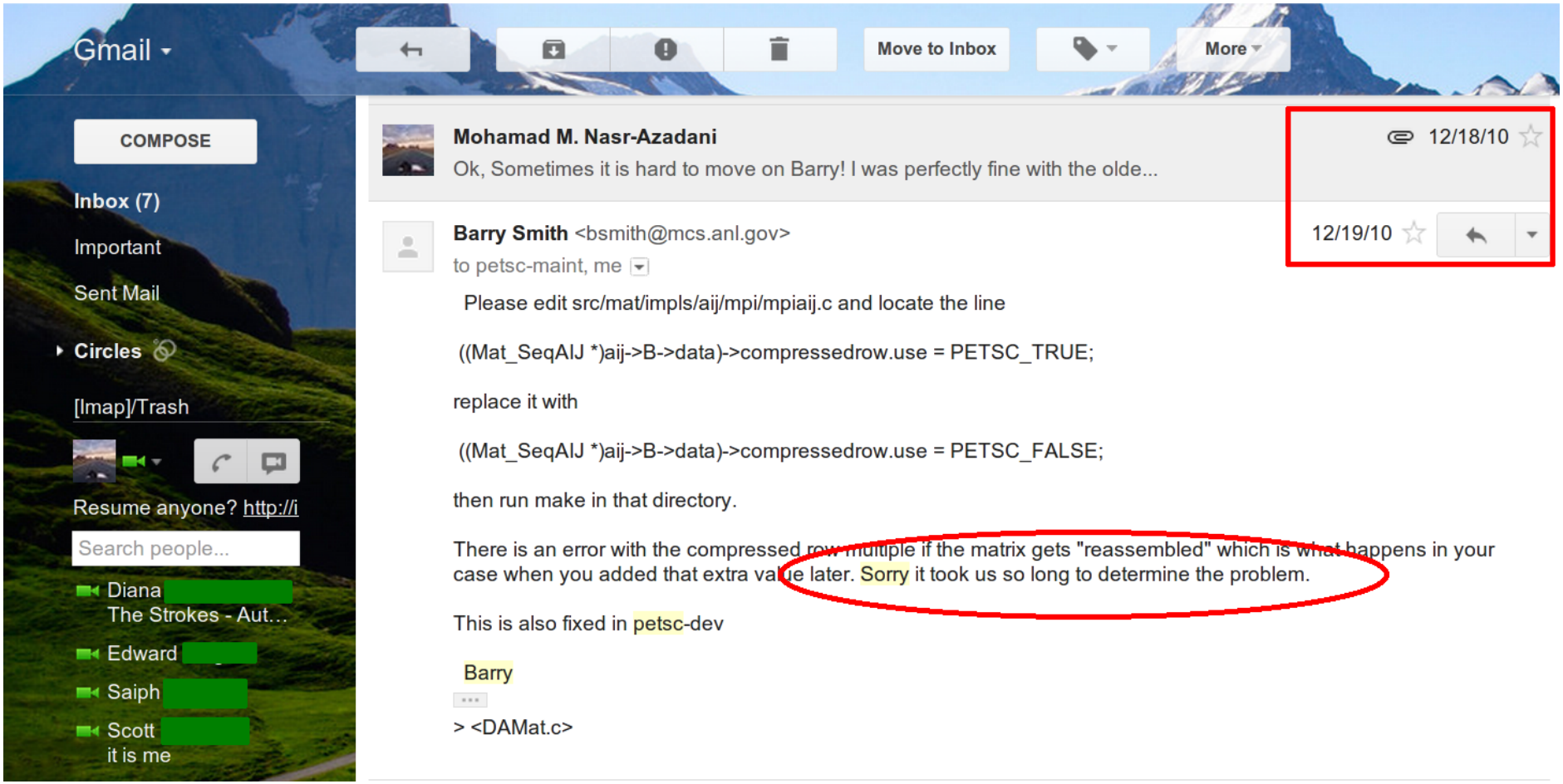
What is PETSc?

- Definition: Portable Extendable Toolkit for Scientific Computations
- It essentially contains: Parallel PDE linear/nonlinear algebraic tools and **solvers**
- Hides **99%** of the need to run MPI commands (parallelism)
- Interfaces to many many other numerical packages
- It is extremely well-supported (an ongoing project)

What is PETSc?



What is PETSc?



What does PETSc target?

- Serial and Parallel
- Linear and nonlinear
- Finite difference and finite element
- Structured and unstructured

What does PETSc NOT target?

- Sophisticated visualization
- Discretize PDE's or ODE's
- Load balancing
- Grid generation, etc

PETSc can be used with:

- C/C++ (originally written in C)
- Fortran
- Some: Python and MATLAB interface

PETSc's basic objects

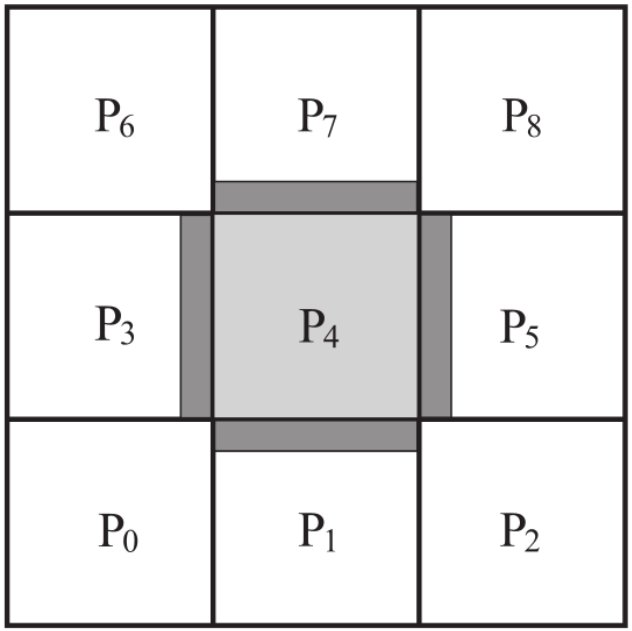
- Mat (matrix)
- Vec (vector)
- KSP (solver), [PC (preconditioners)]
- SNES (nonlinear solver)
- TS (time stepping)

Variable declarations, C

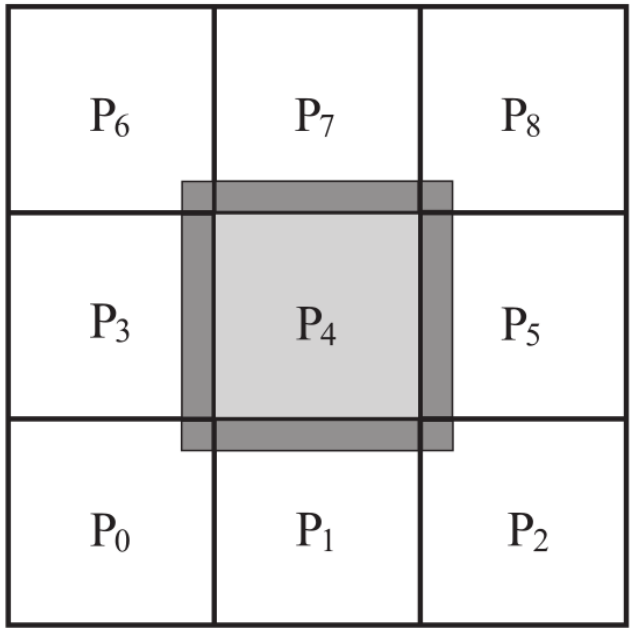
```
int main(int argc, char **argv) {
        KSP solver;
        Mat A;
        Vec x, y;
        PetscInt size = 10;
        PetscScalar value = 1.0;
        double extra = value*2.0;
          .
          .
```

Distributed arrays (DMDA)

- Very powerful tool: Structured orthogonal grids (1D, 2D, and 3D)
- Allows you to use (i,j,k) index in data arrays
- Hides the complexity associated with updating ghost nodes



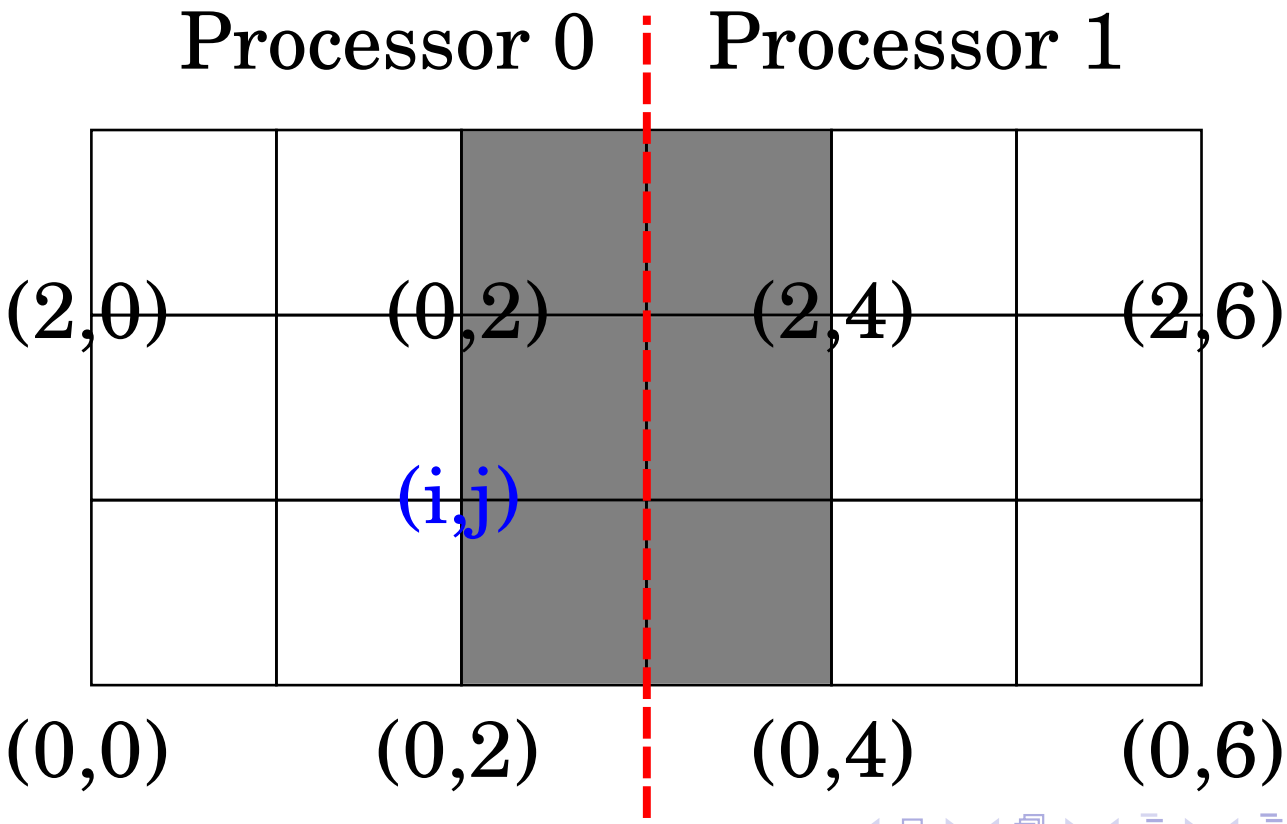
(a) Star stencil



(b) Box stencil

Distributed arrays (DMDA)

- Major benefit: User can still employ data arrays in **(i,j,k)** format using **global indexing** rules
- Hides the complexity of ghost nodes and communication betweent processors



Distributed arrays (DMDA)

- Tell PETSc about your data array size, boundary condition, ...

```
DMDACreate2d(some arguments, DM *dm);
```

- Automatically defines the matrix structure

```
DMCreateMatrix(DM dm, const MatType mtype, Mat *mat);
```

- Automatically creates vectors (data arrays) associated with the parallel layout

```
DMCreateGlobalVector(DM dm, Vec *vec);
DMCreateLocalVector(DM dm, Vec *vec);
```

DMDA Matrix

- Use this command to insert values at any given (i,j,k)

```
MatSetValuesStencil(Mat mat, some arguments);
```

DMDA Vector

- Use this command to access (read/write) vector data in (i,j,k) format

```
DMDAVecGetArray(DM da, Vec vec, void *array)
```

- Once operations are done, CALL this function to restore the vector

```
DMDAVecRestoreArray(DM da, Vec vec, void *array)
```

Example: Poisson equation

- The Poisson equation of the form

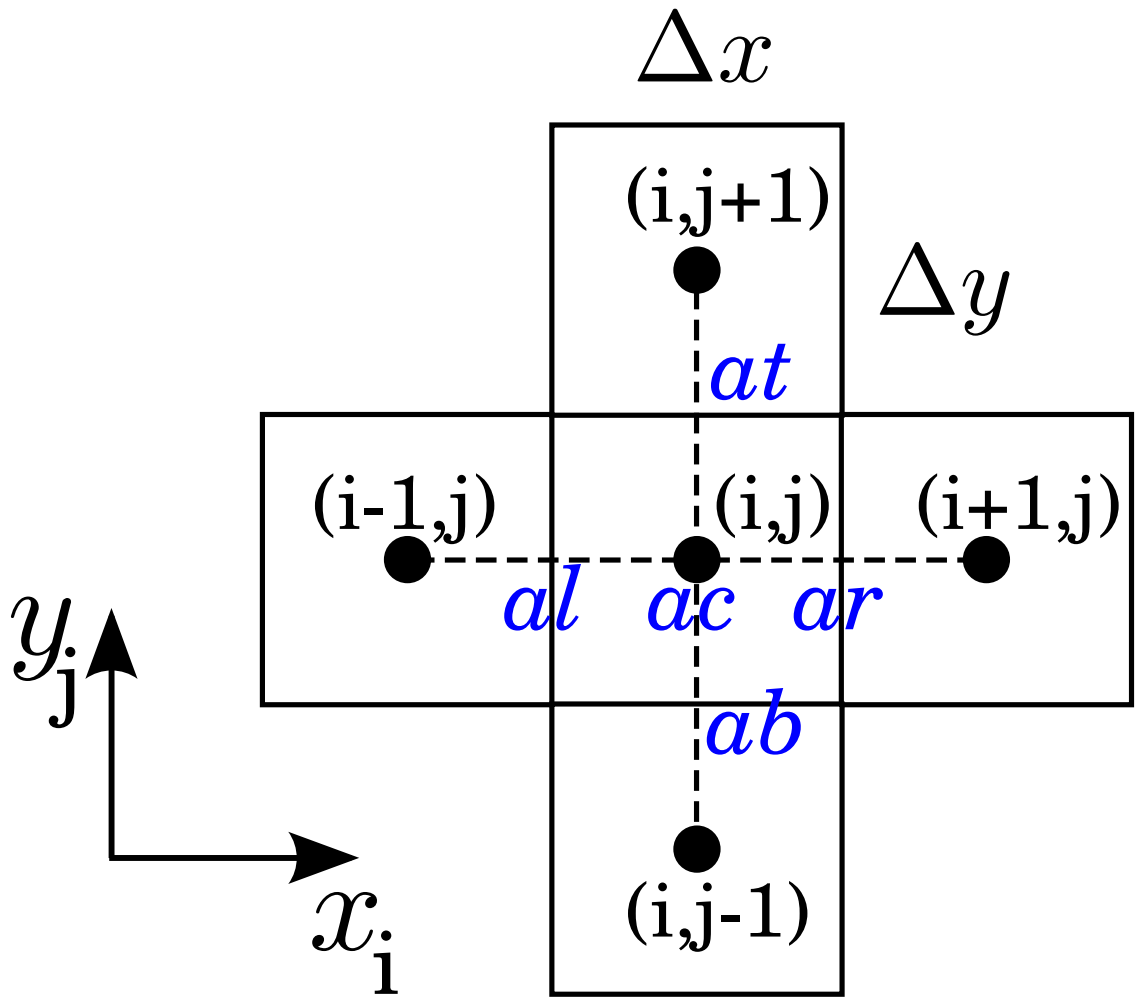
$$\nabla^2 q = f(x,y) \qquad 0 \le x \le 1\,, \quad 0 \le y \le 1.$$

- Discretization on a uniform grid via 2^{nd}-order finite difference scheme

$$\frac{q_{i+1,j} - 2q_{i,j} + q_{i-1,j}}{\Delta x^2} + \frac{q_{i,j+1} - 2q_{i,j} + q_{i,j-1}}{\Delta y^2} = f_{i,j}$$

Example: Discretization

- Connectivity and 5-point numerical stencil



Example: Matrix setup

- Connectivity and 5-point numerical stencil

```
MatStencils row_index, col_indices[5];
PetscScalar coefficients[5];
/* center node index (i,j) and coefficient, ac */
col_indices[0].i = i;
col_indices[0].j = j;
coefficients[0] = ac;
/* right node index (i+1,j) and coefficient, ar */
col_indices[1].i = i+1;
col_indices[1].j = j;
coefficients[1] = ar;
```

Example: Matrix setup

```
/* left node index (i-1,j) and coefficient, al */
   col_indices[2].i = i-1;
   col_indices[2].j = j;
   coefficients[2] = al;
         .
         .
/* And of course the row index is also needed */
   row_index.i = i; row_index.j = j;
/* Now, insert the coefficients */
   MatSetValuesStencil(A, 1, &row_index, 5, col_indices, coefficients,
INSERT_VALUES);
```

Example: Poisson equation

- The Poisson equation of the form

$$\nabla^2 q = f(x,y) \qquad 0 \le x \le 1\,, \quad 0 \le y \le 1.$$

- Discretization on a uniform grid via 2^{nd}-order finite difference scheme

$$\frac{q_{i+1,j} - 2q_{i,j} + q_{i-1,j}}{\Delta x^2} + \frac{q_{i,j+1} - 2q_{i,j} + q_{i,j-1}}{\Delta y^2} = f_{i,j}$$

Example: Right-hand-side setup

```
PestcScalar **f;
Vec b;
DM da;
      .
      .
DMDAVecGetArray(da, b, &f);
/* Insert the rhs_value for current index at (i,j) */
f[j][i] = rhs_func(x,y);
      .
      .
DMDAVecGetArray(da, b, &f);
```

Example: KSP solver

- PETSc provides ksp (iterative) solvers with various preconditioners.
- Black box solvers!
- Pass matrix and right-hand-side vectors

```
KSP solver;
Mat M;
Vec b, x;
      . /* Setup LHS matrix (M) and RHS (b) vector */
      .
KSPCreate(PETSC_COMM_WORLD, &solver);
KSPSetOperators(solver, M, M, SAME_PRECONDITIONER);
KSPSetFromOptions(solver);
KSPSolve(solver, b, x);
```

PETSc pseudo code

```
static char help[] = "Hello world PETSc!";
#inlcude "petsc.h"
int main(int argc, char **argv) {

      PetscErrorCode ierr;
/* Always start your program with this command */
      ierr = PetscInitialize(&argc, &argv,(char*)0, help);
      CHKERRQ(ierr); /* Error checking for PETSc functions */
           .
/*PETSc variables and function calls */.
           .
      ierr = PetscFinalize();
      return 0;
}
```

Example: Hello world

- Using **PetscPrintf()** and **PetscSynchronizedPrintf()**
- Let's run code ex0.c

```
make ex0
./ex0
```

- Now, let's run it on 4 processors

```
mpiexec -np 4 ./ex0
```

Example: 2-D Poisson equation

- After discretization, the resulting linear system is to be solved by an iterative solver.

$[A]\ \{q\} = \{b\}$
[A]: Penta-diagonal symmetric matrix

- We need:

Distributed array context **DMDA DA2d;**
LHS matrix **Mat LHS_mat;**
RHS vector **Vec RHS_vec_g;**
Solution vector **Vec Sol_vec;**

- Pass the setup matrix and RHS vector to solver

KSP iterative solver **KSP solver;**

Example: 2-D Poisson equation

- Pass input parameters (Nx,Ny) and boundary conditions (bc: 1 for **Neumann**, 2 for **Dirichlet**) via command line arguments

```
make ex1
./ex1 -Nx 10 -Ny 10 -bc 1
```

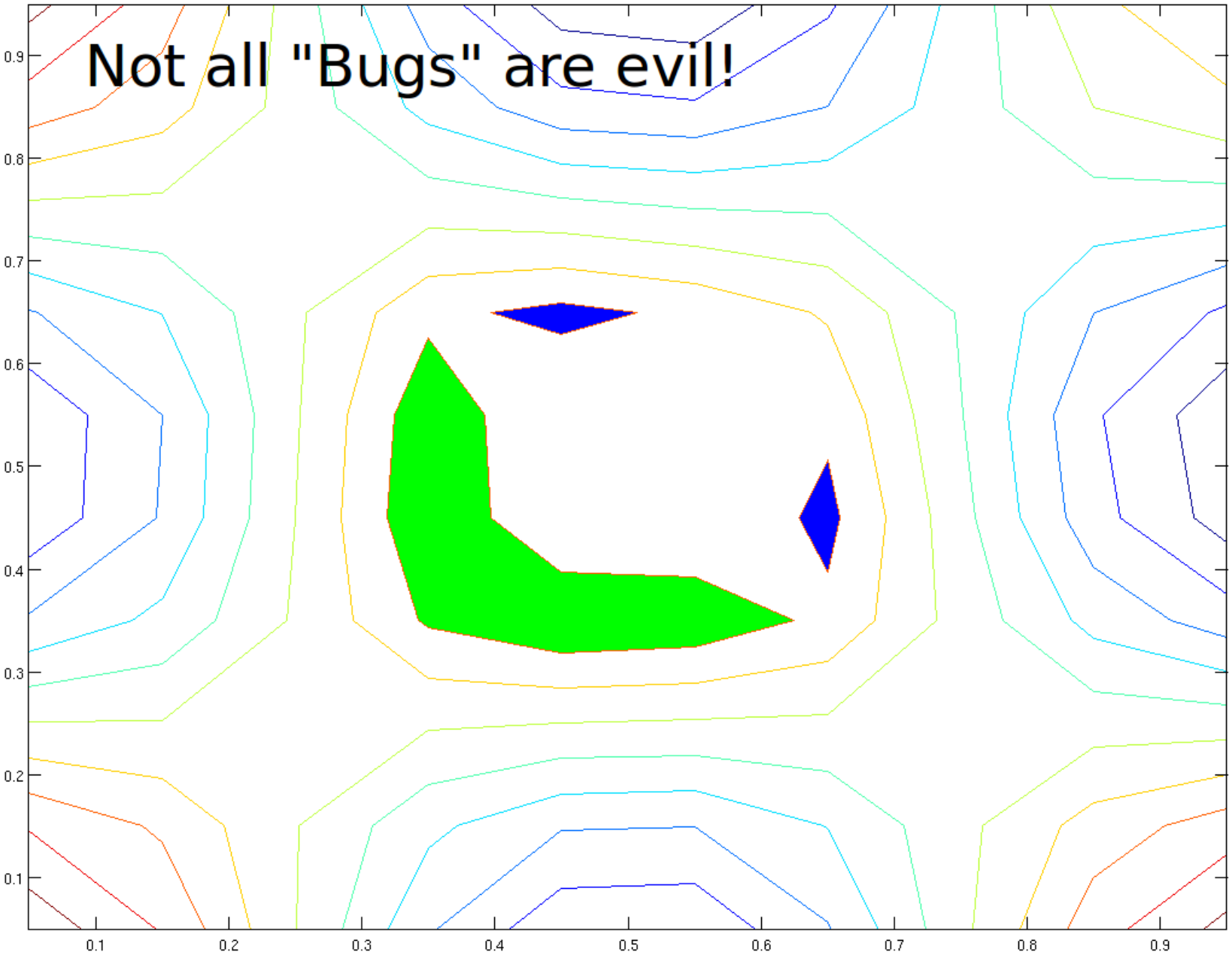
- Now, let's run it on 4 processors

```
mpiexec -np 4 ./ex1 -Nx 10 -Ny 10 -bc 1
```

- Compare:
  - Number of iterations used for convergence
  - Errors (E1, and E2)

Find more information

- Official website: `http://www.mcs.anl.gov/petsc/`
- Email lists:
  - `petsc-users@mcs.anl.gov`
  - `petsc-maint@mcs.anl.gov`
- Or email me: `mmnasr@engineering.ucsb.edu`


Not all "Bugs" are evil!
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9