# A first PDE solution in PETSc

## Finite differences on a structured grid

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# outline for today

book Chapter 2:

- finish up the `tri.c` example (*only 2 slides*)

book Chapter 3:

- boundary-value problem for Poisson's equation:

$$-\nabla^2 u = f$$

- finite difference (FD) method
- FD method generates linear system $A\mathbf{u} = \mathbf{b}$

# large (merely tridiagonal) linear system

- look at `c/ch2/tri.c`; notice
  - `PetscOptions...()`
  - `MatGetOwnershipRange(A,&Istart,&Iend)`
  - generic row of $A$ is

$$-1 \quad 3 \quad -1$$

  - "manufacture" exact solution: `MatMult(A,xexact,b)`
- for example, use Richardson as `KSP`:

```
$ ./tri -ksp_monitor -ksp_type richardson \
    -pc_type none
$ ./tri -ksp_monitor -ksp_type richardson \
    -pc_type jacobi
```

- performance = execution time, for now

```
$ time ./tri -tri_m 10000
$ alias timer
$ timer ./tri -tri_m 10000
```

# performance on $m = 2 \times 10^7$ unknowns

```
$ timer mpiexec -n N ./tri -tri_m 20000000 \
    -ksp_rtol 1.0e-10 -ksp_type KSP -pc_type PC
```

| KSP | PC | N=1 time (s) | N=4 time (s) |
|---|---|---|---|
| preonly | lu | 10.74 | |
| | cholesky | 5.84 | |
| richardson | jacobi | 13.48 | 5.45 |
| gmres | none | 9.99 | 5.30 |
| | jacobi | 10.23 | 4.49 |
| | ilu | 4.77 | |
| | bjacobi+ilu | | 2.99 |
| cg | none | 7.22 | 3.18 |
| | jacobi | 7.49 | 3.31 |
| | icc | 4.81 | |
| | bjacobi+icc | | 2.87 |

Table 2.2: Times for `tri.c` to solve systems of dimension $m = 2 \times 10^7$. In this case the matrix is *tridiagonal*, *symmetric*, *diagonally-dominant*, and *positive definite*. All runs were on WORKSTATION (see page 41).

note: for `N`$>1$ use

```
-pc_type bjacobi -sub_pc_type PC
```

if you want `PC=ilu,icc` on each process

# Poisson equation on a square

- let $\mathcal{S}$ be the open unit square $(0, 1) \times (0, 1)$
- recall *Laplacian* of $u(x, y)$:

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$$

- boundary value problem:

$$\begin{aligned} -\nabla^2 u = f \quad & \text{on } \mathcal{S} \\ u = 0 \quad & \text{on } \partial\mathcal{S} \end{aligned}$$

- for example, if

$$\begin{aligned} f(x, y) = 2(1 - 6x^2)y^2(1 - y^2) \\ + 2(1 - 6y^2)x^2(1 - x^2) \end{aligned}$$

then $u(x, y) = (x^2 - x^4)(y^4 - y^2)$

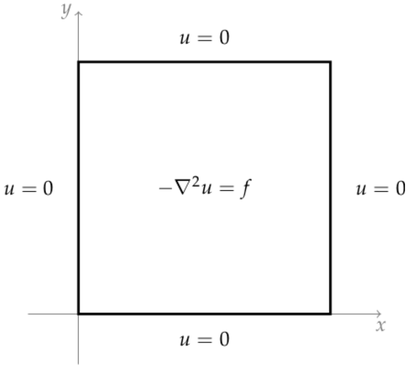



Figure 3.1: The Poisson equation on the unit square $\mathcal{S}$, with homogeneous Dirichlet boundary conditions.

# where does Poisson come from?

- model for: electrostatic potential, equilibrium distribution from random walks, various other physical phenomena
- for example, heat conduction in solids:
  - if $k$ is the conductivity then Fourier's law says heat flux is
    $$\mathbf{q} = -k\nabla u$$
  - if $f$ describes a heat source then energy conservation says
    $$c\rho\,\partial u/\partial t = -\nabla \cdot \mathbf{q} + f$$
  - if $k = 1$, and in equilibrium (steady state) then get our Poisson equation
    $$0 = \nabla^2 u + f$$

# choice of grid = first step of an approximation

- put *structured grid* of $m_x$ by $m_y$ points on $\mathcal{S}$
- spacing $h_x = 1/(m_x - 1)$ and $h_y = 1/(m_y - 1)$
- grid coordinates are $x_i = i\, h_x$, $y_j = j\, h_y$
- *the main notation of numerical differential equations*: the unknown value of $u(x, y)$ at node $(x_i, y_j)$ will be approximated by the numbers $u_{i,j}$ which we actually compute:

$$u_{i,j} \approx u(x_i, y_j)$$

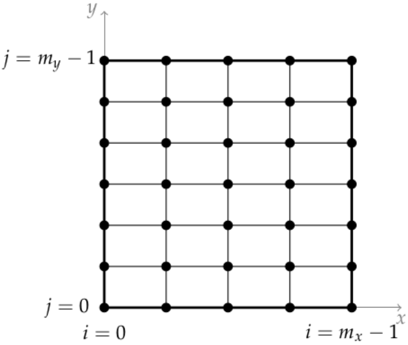



Figure 3.2: A grid on the unit square $\mathcal{S}$, with $m_x = 5$ and $m_y = 7$.

# finite difference approximation of partial derivatives

- our equation has second partial derivatives
- steps to the finite difference form of the Laplacian:

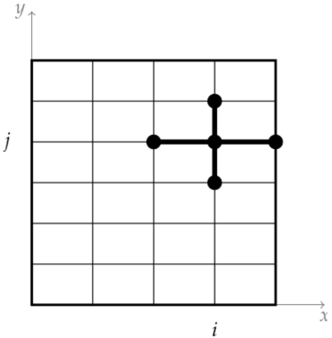
$$\frac{\partial u}{\partial x}(x,y) = \lim_{h\to 0} \frac{u(x+h,y)-u(x,y)}{h}$$

$$\frac{\partial u}{\partial x}(x_i,y_j) \approx \frac{u(x_i+h_x,y_j)-u(x_i,y_j)}{h_x}$$

$$\approx \frac{u_{i+1,j}-u_{i,j}}{h_x}$$

$$\frac{\partial^2 u}{\partial x^2}(x_i,y_j) \approx \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h_x^2}$$

$$\nabla^2 u(x_i,y_j) \approx \frac{u_{i+1,j}-2u_{i,j}+u_{i-1,j}}{h_x^2} + \frac{u_{i,j+1}-2u_{i,j}+u_{i,j-1}}{h_y^2}$$




“stencil” ↗

# FD scheme gives linear system

- FD equations for our Poisson problem:

$$-\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h_x^2} - \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h_y^2} = f_{i,j},$$

$$u_{0,j} = 0, \quad u_{m_x-1,j} = 0, \quad u_{i,0} = 0, \quad u_{i,m_y-1} = 0$$

  - first equation applies at all interior points
  - boundary condition treated as trivial equations: "1 $u = 0$"
- is a linear system of $L = m_x m_y$ equations in $L$ unknowns

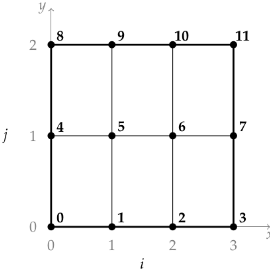
$$A\mathbf{u} = \mathbf{b}$$

where $A$ is $L \times L$ matrix and $\mathbf{u}, \mathbf{b}$ are $L \times 1$ column vectors

# ordering of unknowns

- actually building linear system requires global ordering of unknowns: $k = 0, 1, \dots, L$
- $m_x = 4$ and $m_y = 3$ case has $L = 12$:

$$
\begin{bmatrix}
1 & & & & & & & & & & & \\
 & 1 & & & & & & & & & & \\
 & & 1 & & & & & & & & & \\
 & & & 1 & & & & & & & & \\
 & & & & 1 & & & & & & & \\
 & c & & & b & a & b & & & c & & \\
 & & c & & & b & a & b & & & c & \\
 & & & & & & & 1 & & & & \\
 & & & & & & & & 1 & & & \\
 & & & & & & & & & 1 & & \\
 & & & & & & & & & & 1 & \\
 & & & & & & & & & & & 1
\end{bmatrix}
\begin{bmatrix} u_{0,0} \\ u_{1,0} \\ u_{2,0} \\ u_{3,0} \\ u_{0,1} \\ u_{1,1} \\ u_{2,1} \\ u_{3,1} \\ u_{0,2} \\ u_{1,2} \\ u_{2,2} \\ u_{3,2} \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ f_{1,1} \\ f_{2,1} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
$$




  - only $k = 5, 6$ eqns are *not* b.c.s

- (weak) diagonal dominance: $a = |2b + 2c|$
- *but* matrix is not symmetric
- surprisingly-large condition number for small example: $\kappa(A) = 43.16$