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High Performance Computing 2

SoSe 2017

Sheet 1

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Hints:

1) Attendance to the exercises will be a necessary condition for the exam.
2) In every exercise, there will be a short colloquium (oral exams), where the last exercise will be discussed.
   a) Each colloquium will be around 5-10 min.
   b) The goal of the colloquium will be to discuss the previous topics and exercises.
   c) Each colloquium is either passed or failed. 50% of the colloqiums have to be passed for the permission to attend the exam, which will be a project.

Introduction

In this exercise we want to consider the Poisson equation, which reads

$$\begin{aligned} -\Delta u &= f \qquad \text{in } \Omega \\ u &= 0 \qquad \text{on } \Gamma := \partial\Omega. \end{aligned}$$

For simplicity, we consider $u \in C^4(\Omega), \Omega = (0,1) \times (0,1), f = 1$. This problem represents a simple diffusion model for the temperature distribution $u(x,y)$ in a square plate. The exact solution in this case is known and reads

$$u(x,y) = \frac{1-x^2}{2} - \frac{16}{\pi^3} \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \left\{ \frac{\sin(k\pi(1+x)/2)}{k^3 \sinh(k\pi)} \Big(\sinh(k\pi(1+y)/2) + \sinh(k\pi(1-y)/2) \Big) \right\}.$$

In this exercise, we want to consider and analyze the finite difference approximation of the above given poisson equation. Given an integer $N \geq 1$, we construct rectangular grids $\mathcal{T}_h$ by the tensor product of a grid of the interval $(0,1)$ by $\{x_i = i\,h, i = 0,\ldots,N+1,\, h = 1/(N+1)\}$, h be the mesh-size of $\mathcal{T}_h$. We denote $\Omega_h = \{(x_i,y_j) \in \Omega\}$ and boundary $\Gamma_h = \{(x_i,y_j) \in \Gamma\}$. We consider the discrete function space given by $V_{h,0} = \{u_h(x_i,y_j), 1 \leq i,j \leq N\}$. Further, for the sake of simplicity we denote $u_{i,j} := u_h(x_i,y_j) \approx u(x_i,y_j)$. It is fairly standard to approximate the Laplace operator at an interior node (x_i,y_j) with the centered second difference, which reads

$$\begin{aligned} (\Delta_h)_{i,j} &= (D^2_{xx})_{i,j} + (D^2_{yy})_{i,j} \\ &= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2} \\ &= \frac{u_{i+1,j} + u_{i,j+1} - 4u_{i,j} + u_{i-1,j} + u_{i,j-1}}{h^2} \end{aligned}$$

It is called the five point stencil since only five points are involved and $-(\Delta_h)_{i,j}$ can be denoted by the following stencil symbol

$$\begin{pmatrix} & -1 & \\ -1 & 4 & -1 \\ & -1 & \end{pmatrix}$$

For the right hand side, we simply take node values, i.e. $f_{i,j} = f(x_i, y_j)$. The finite difference methods for solving Poisson equation with homogeneous boundary conditions then reads

$$-h^2 \cdot (\Delta_h)_{i,j} = h^2 \cdot f_{i,j} \quad (1 \leq i, j \leq N)$$

Let us consider an ordering of $n = N^2$ grids and use a single index $k \in \{1, \ldots, n\}$ for $u_k = u_{i(k),j(k)}$. In Figure 1 four different mapping $k \to (i(k), j(k))$ are illustrated. With any choosing ordering the discretized poisson problem can be written as a linear system of equations

$$Au = f$$

where $A \in \mathbb{R}^{n \times n}$, $u \in \mathbb{R}^n$, and $u \in \mathbb{R}^n$.
Now, the obvious problem is how to order the nodes of the grid. We present the following possibilities

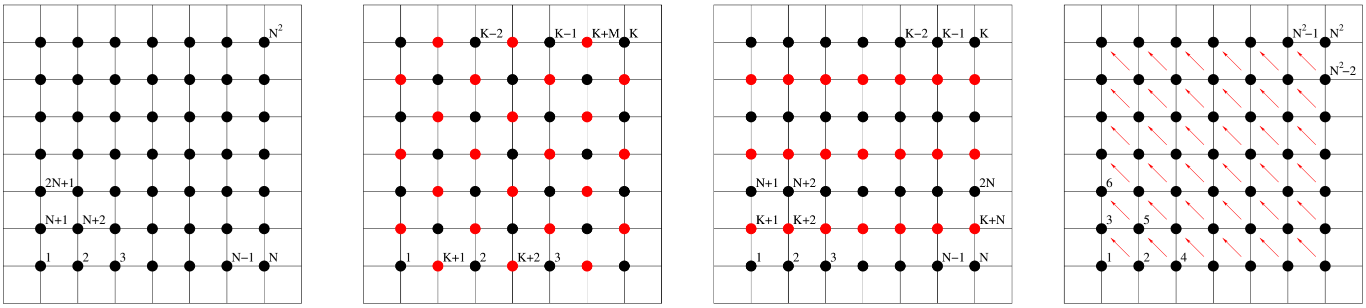

Abbildung 1: Different ordering of nodes of a square grid. Lexicographical (row) ordering (left), red-black ordering (middle left), zebra (row) ordering (middle right), and diagonal ordering (right).

Exercise

1. Which structure takes the matrix A, if we consider the one-dimensional poisson problem, i.e. on $\Omega = (0, 1)$, with homogeneous Dirichlet boundary conditions? Show, that A is given by

$$A := \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \tag{1}$$

2. Which structure takes the matrix A, if we consider the one-dimensional poisson problem, i.e. on $\Omega = (0, 1)$, with homogeneous Dirichlet boundary conditions on $x = 0$ and Neumann boundary conditions on $x = 1$, i.e.

$$\begin{aligned} -u_{xx} = f \qquad & x \in (0, 1) \\ u(0) = 0, \qquad & \frac{\partial}{\partial x} u(1) = 0. \end{aligned}$$

Show, that A is now given by

$$A := \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix} \tag{2}$$

Hint: Use $\frac{\partial}{\partial x} u(1) = \frac{\partial}{\partial x} u(x_N) \approx \frac{u(x_{N+1}) - u(x_{N-1})}{2h}$ with a fictive point x_{N+1}.

3. The matrices from 1. and 2. are called Toeplitz matrices. For the eigenvalues of matrix (1) it can be shown, that

$$\lambda_k(A) = 4\Big(\sin^2\big(\frac{\pi}{2}\frac{k}{n+1}\big)\Big)$$

and for the eigenvalues of the matrix (2)

$$\lambda_k(A) = 4\Big(\sin^2\big(\frac{\pi}{2}\frac{k-1}{n}\big)\Big), \quad (k \in \{1, \ldots, n\}).$$

a) What does this mean for the condition number of both matrices?

b) What consequences does this have for solving the linear system of equations?

c) Write a matlab code, which computes the eigenvalues from exercise 1. and 2. Compare them with the exact eigenvalues. Verifiy your statements of a) and b).

4. Show, that for the lexicographic ordering the coefficient matrix for the two-dimensional poisson problem takes the form of a block-tridiagonal matrix :

$$A = \begin{pmatrix} T & -I & & & \\ -I & T & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & T & -I \\ & & & -I & T \end{pmatrix} \tag{3}$$

built from $N \times N$ blocks T, which again are tridiagonal $N \times N$ matrices, and I is the $N \times N$ identity matrix, i.e.

$$T := \begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix}, \quad I := \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix}.$$

For the 'zebra'-ordering and even N, the matrix A has also a structure consisting of three block diagonals.

$$A = \left(\begin{array}{ccc|ccc} T & & & -I & & \\ & \ddots & & & \ddots & \\ & & T & & & -I \\ \hline -I & & & T & & \\ & \ddots & & & \ddots & \\ & & -I & & & T \end{array}\right).$$

5. Which structure has the matrix for the red-black ordering and for the diagonal ordering?

6. Let $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{p\times q}$. The the Kronecker product (or tensor product) of A and B is defined as the matrix

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{pmatrix} \in \mathbb{R}^{mp\times nq}.$$

a) Calculate $T \otimes I$ and $I \otimes T$.

b) For the lexicographic ordering the discrete Laplacian in d dimension is a Kronecker sum of 1D discrete Laplacians. From this representation, we get easily knowledge of the eigenvalues of A by the eigenvalues of T, i.e. let $A \in \mathbb{R}^{n\times n}$ have eigenvalues λ_i, $i \in \{1, \ldots, n\}$, and let $B \in \mathbb{R}^{m\times m}$ have eigenvalues μ_j, $j \in \{1, \ldots, m\}$. Then the Kronecker sum $A \oplus B := (I_m \otimes A) + (B \otimes I_n)$ has mn eigenvalues,

$$\lambda_1 + \mu_1, \ldots, \lambda_1 + \mu_m, \lambda_2 + \mu_1, \ldots \lambda_2 + \mu_m, \ldots, \lambda_n + \mu_m .$$

What are the consequences fror the matrix given in (3)?

c) Write a matlab code, which computes the eigenvalues of the matrix (3). Verify numerically the statement from b). What are the consequences for the condition number of A in this case and for solving the linear system of equations?

7. Write a matlab function, which solves the two-dimensional poisson problem on $\Omega = (0, 1)^2$ and for arbitrary f and homogenous Dirichlet boundary conditions. You can use the well-known backslash operator. Plot your solution for various h.

Hints: You can use the matlab functions `eigs` for computing the eigenvalues of matrices given in sparse format and `kron` for computing the tensor product of two matrices.