Computer exercise for WI4201
A Comparison of Sparse Direct and Preconditioned Krylov Subspace Solvers in Two and Three Dimensions

Students: Group:
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Guidelines

- The deadline to hand in the report on this assignment is **January 15th, 2021**.
- Make sure to schedule an intermediate video-call appointment with your supervisor Merel Schalkers (email: M.A.Schalkers@tudelft.nl) in the **first week of December (6th of December till 10th of December)** where you can discuss your progress with this take-home exam. The minimal implementation results you have to show are: the convergence to the exact solution and the implementation of the first solver required in your take home exam. It is allowed that only one of you comes to the appointment if the other is not available at the same time.
- We accept both hand-written (note that you will have to scan your report) and computer-written (using Word, Latex or other) reports.
- Put your group number and the project letter on the front page of your report.
- Due to current measures, delivering the hard copy of your reports is no longer possible. Please send us your reports **via email**.
- For the computer implementation, any language can be used (Matlab, Python or other).
- The implementation itself will **NOT** be graded. All intelligence and wisdom in realizing the implementation should therefore be reflected in the report.
- Write a concise report in which you answer the questions one by one. Both the structure of the report and the correctness of the answers will be taken into account in the grade. Do include the source code of your implementation in this report.

The goal of this assignment is to compare the performance of some sparse direct and iterative solution methods applied the discrete Laplacian in two and three dimensions. In this assignment the Poisson problem on the unit square $\Omega = [0,1]^2$ and the unit cube $\Omega = [0,1]^3$ is considered. The Poisson equation relates the unknown field $u(\mathbf{x}) = u(x,y)$ in 2D ($u(\mathbf{x}) = u(x,y,z)$ in 3D) to the known excitation $f(\mathbf{x})$:

$$-\Delta u = -\text{div} \cdot \text{grad}\, u = f \text{ on } \Omega\,. \tag{1}$$

We supply this problem with non-homogeneous Dirichlet boundary conditions:

$$u = u_0 \text{ on } \partial\Omega. \tag{2}$$

Assume that the computational domain Ω is discretized by a uniform mesh denoted by Ω^h with n elements and meshwidth $h = \frac{1}{n}$ in each direction. Assume that a central second order accurate finite difference scheme (5-point scheme in 2D and a 7-point scheme in 3D) is applied to discretize the partial differential equation (1) supplied with (2) and assume that the boundaries are **not** eliminated from the linear system (cfr. Lecture Notes). The discretization then leads to a linear system for the discrete solution $\mathbf{u}^h$:

$$A^h \mathbf{u}^h = \mathbf{f}^h \tag{3}$$

for which the coefficient matrix A^h has a number of desirable properties. Let $\mathbf{u}^h_{ex}$ denote the exact solution evaluated in the grid nodes.

We will solve this problem with several different solvers. We will first look into direct solvers for the system (3). The Cholesky decomposition of a matrix A^h can be written as

$$A^h = C^h (C^h)^T . \tag{4}$$

Another way is to use Symmetric Successive Overrelaxation (SSOR) as a basic iterative method (BIM). Given a zero initial guess for $\mathbf{u}^h$ and denoting the iteration index as m, solve linear system (3) until convergence criterion

$$\frac{\|\mathbf{r}_m\|_2}{\|\mathbf{f}^h\|_2} \leq 10^{-10} \tag{5}$$

is met.

Lastly, one can use Symmetric SOR as a preconditioner for the conjugate gradient (CG). Use the reader and other literature for information about these methods.

Answer each question in this assignment for both the 2D and 3D problem unless it is stated otherwise.

Pen and Paper Assignments (50 points)

1. *(4 pt)* Determine the source function $f(\mathbf{x})$ and the boundary data $u_0(\mathbf{x})$ such that $u_{ex}(\mathbf{x}) = \sin(xy)$ in 2D (and $u_{ex}(\mathbf{x}) = \sin(x\,y\,z)$ in 3D) is the exact solution to the problem.
2. *(5 pt)* Give the size, sparsity structure and upper and lower bandwidth of the matrix A^h.
3. *(3 pt)* Motivate why a Cholesky decomposition can be used to solve the system.
4. *(10 pt)* Derive an expression for the computational complexity of factorization and forward/backward solving, as a function of problem size N, taking matrix structure into account.
5. *(5 pt)* Describe SSOR as a BIM and motivate why it can be used to solve the system considered.
6. *(9 pt)* Derive an expression for the complexity of one single iteration of the algorithm. Assuming `Niter` iterations are required, derive an estimate for the complexity to iterate until convergence.
7. *(14 pt)* Repeat the questions 5. and 6. using SSOR as a preconditioner

Implementation Assignments (50 points)

1. *(5 pt)* Implement a code that constructs the matrix A^h and the right-hand side vector $\mathbf{f}^h$.
2. *(8 pt)* Solve the linear problem by a direct solver for $h = \frac{1}{2^p}$ for $p = 2, \ldots, 10$ in 2D (and $p = 2, \ldots, 8$ in 3D) and verify that the discretization scheme is second order accurate by inspecting the max-norm of the discretization error $||\mathbf{u}^h - \mathbf{u}^h_{ex}||_\infty$.

   Coding Assistance:

- For the construction of A^h: first construct A^h for the 1D problem on $\Omega = [0, 1]$ and subsequently use the tensor products to construct A^h in 2D and 3D.

3. *(5 pt)* Report on the CPU time required for the factorization and forward/backward linear solving using eq. (4) as function of the problem size. Use to this end the same sequence of meshes as in the previous section. Compare with theoretical estimates and draw conclusions.

4. *(5 pt)* Let $nnz(A)$ denote the number of nonzeros in the matrix A. Report on the fill-in ratio defined as $nnz(C)/nnz(A)$ as a function of problem size N. Explain how this fill-in relates to the performance of the direct solver.

5. *(4 pt)* Introduce a matrix reordering scheme that reduces the bandwidth, repeat the two tests above and draw again conclusions.

6. *(5 pt)* Solve the linear system using SSOR with parameter $\omega = 1.5$ used as a BIM. For various values of N, make a logarithmic plot of $\frac{\|\mathbf{r}_m\|_2}{\|\mathbf{f}^h\|_2}$ versus m.

7. *(5 pt)* For various values of N, report on the asymptotic rate of convergence by tabulating the residual reduction factor $\frac{\|\mathbf{r}_m\|_2}{\|\mathbf{r}_{m-1}\|_2}$ during the last five iterations.

8. *(4 pt)* Report on CPU time required to solve the linear system using SSOR as a BIM and compare these number with both theoretical estimates and the CPU time required by direct solvers.

9. *(5 pt)* Solve the linear system using SSOR used as a preconditioner for the CG. For various values of N, make a logarithmic plot of $\frac{\|\mathbf{r}_m\|_2}{\|\mathbf{f}^h\|_2}$ versus m, compare these graphs with those in the previous section and draw conclusions.

10. *(4 pt)* Report on CPU time required to solve the linear system using SSOR as a preconditioner and compare these number with both theoretical estimates, the CPU time required by direct solvers and SSOR as a basic iterative scheme.