



Homework Assignment 11

Please submit the following files as indicated below: source code PDF file image file video file

Even though the lion share of the computational expense when solving a PDE is the solution of the discrete linear system $Ax = b$, we have never spent a lot of thought on how to solve these systems. So far, we have simply used some high-level commands like the backslash in GNU Octave / MATLAB and `solve` in FEniCS. These commands would first run some initial tests to try and detect certain structure in the matrix, and then they choose a suitable method.

This can be done more efficiently. Since we already have a lot of knowledge about properties of the matrix A , we can select the best possible solver ourselves so that no additional testing is necessary at runtime.

Therefore, you will now learn about numerical methods for solving linear systems that stem from discretisations of PDEs. To choose a method that is (i) guaranteed to converge and (ii) as efficient as possible, you will have to use all your knowledge about the matrix A .

Question 1 considers *direct solvers*, which are useful for linear systems of moderate size, e.g. discretised 1D or 2D PDEs. Question 2 deals with *iterative solvers*, which are needed for very large systems, e.g. from 3D PDE problems.

Question 1 | 2 marks | Read about LU factorisation (aka Gaussian elimination) and CHOLESKY factorisation.

(a) Which of these direct solvers is most appropriate for solving the two linear systems

$$\left(M^h + (\theta \Delta t c)^2 K^h\right) \vec{u}_+^h = M^h (\vec{u}_o^h + \Delta t \vec{v}_o^h) - \left(\theta (1 - \theta) (\Delta t c)^2\right) K^h \vec{u}_o^h \quad (1a)$$

$$M^h \vec{v}_+^h = M^h \vec{v}_o^h - \Delta t c^2 K^h (\theta \vec{u}_+^h + (1 - \theta) \vec{u}_o^h) \quad (1b)$$

in the finite-element discretisation of the wave equation (cf Assignment 10) and why?

- CHOLESKY factorisation:

CPU requirements $\sim \frac{1}{3}n^3$ operations

RAM requirements matrix L

Applicability works for symmetric and positive definite matrices only

Conclusion relatively cheap for small to medium size matrices, in particular if multiple linear systems are solved with the same matrix

- LU factorisation:

CPU requirements $\sim \frac{2}{3}n^3$ operations

RAM requirements matrices L and U



Applicability works out of the box for irreducibly diagonally dominant matrices (else partial pivoting may be needed)

Conclusion more expensive, but also more general than CHOLESKY factorisation

\Rightarrow use CHOLESKY factorisation, since the matrices in (1a) and (1b) are both symmetric and positive definite.

- (b) Make a copy of `hw10.py` (you may use the program from the model answers). The new script should integrate the wave equation as in Assignment 10, but it should solve the linear systems with the method you selected in part (a).

Hint: You can find some useful FEniCS commands on the enclosed cheat sheet. Create a solver object for (1a) and another solver object for (1b). Your code should run approximately three times faster than in Assignment 10.

Question 2 | 3 marks |   There are two main classes of iterative solvers: KRYLOV subspace methods and multigrid methods. We will look at KRYLOV subspace methods here.

Read about the conjugate gradient method (CG), the minimal residual method (MINRES) and the generalised minimal residual method (GMRES).

- (a) Which of these iterative solvers is most appropriate for the linear systems in (1) and why?

- CG:

CPU requirements one matrix-vector multiplication per iteration (plus a number of comparably cheap scalar operations)

RAM requirements the current and the immediate past iterate

Applicability works for symmetric and positive definite matrices only

Conclusion very little memory needed, i.e. iterations are cheap even for large matrices

- MINRES:

CPU requirements one matrix-vector multiplication per iteration (plus a number of comparably cheap scalar operations)

RAM requirements the current and the past two iterates

Applicability works for symmetric matrices

Conclusion marginally larger memory requirements than CG, but also applicable to a larger class of matrices

- GMRES:

CPU requirements one matrix-vector multiplication per iteration (plus a number of comparably cheap scalar operations)

RAM requirements the current and all past iterates (i.e. method must be re-started after a certain number of iterations)

Applicability matrices could also be non-symmetric or indefinite

Conclusion significantly more expensive than CG and MINRES, but again more generic

⇒ use CG, since the matrices in (1a) and (1b) are both symmetric and positive definite.

- (b) Modify your FEniCS script from Question 1 to now solve the linear systems with the iterative method you selected in part (a).

Hint: Comment out the lines where you defined the direct solver objects. Create two iterative solver objects instead.

- (c) Iterative methods typically converge significantly faster if they are applied to a preconditioned problem: instead of

$$Ax = b, \tag{2}$$

one solves the mathematically equivalent, but numerically advantageous problem

$$P^{-1}Ax = P^{-1}b. \tag{3}$$

The invertible matrix P , the so-called preconditioner, should on the one hand approximate A as closely as possible, but on the other hand it should be easier to invert than A . Such preconditioners are designed based on the specific properties of the linear system or the original PDE.

Note that if $P \approx A$, then $P^{-1}A \approx \text{id}$. This is what makes (3) more amenable to iterative solvers than (2).

Read about diagonal aka JACOBI preconditioning and incomplete CHOLSKY factorisation. Can you think of an even better preconditioner specifically for the mass matrix M^h than these two generic preconditioners?

The lumped mass matrix \tilde{M}^h is both close to M and trivial to invert since it is diagonal.

NB: The lumped mass matrix actually works so extremely well as a preconditioner that many iterative methods often converge within just three to five (very cheap) iterations!

Your Oral Presentation You can find a worksheet attached to the presentation assignment on **Canvas** which you may want to use to prepare for your talk. Also familiarise yourself with the marking criteria which can be found on the same page to make sure you will cover everything that is needed.

You do not necessarily have to include final results in your talk. If you already have results to share, this is only to your advantage as it allows me to give you some feedback before you submit your written work where they will be graded.

Come up with an interesting title and write a succinct mini-abstract of at most three short sentences. This will also be made available to the public and should thus assume no specialised knowledge, but arouse interest for your talk. Please use the presentation assignment on **Canvas** to submit your title and your mini-abstract.

Your Learning Progress |  What is the one most important thing that you have learnt from this assignment?

Any new discoveries or achievements towards the objectives of your course project?

What is the most substantial new insight that you have gained from this course this week? Any *aha moment*?
