DN3250 - Advanced numerical methods for science and engineering

Goals

This course aims to provide an overview of the modern techniques used in the solution of some of the most common numerical linear algebra problems arising in science and engineering, with special focus on the two topics

1) large linear systems of equations, and
2) large eigenvalue problems.

After the course, you will be able to approach these two problems with the following knowledge:

- Given a matrix/problem with a particular structure you will be able to identify properties important for the choice of algorithm.
- Given the structure of a matrix you will be able to select an appropriate algorithm from the set of common algorithms.
- You should be able to use the selected algorithm by writing a C- or Fortran-program which links it with modern software packages.
- In case of failure of algorithm, you should be able to analyze the output of the algorithm and identify the source of the error and propose one of the typical modifications.

Eligibility and prerequisites

The course is offered to all graduate students at KTH. Basic knowledge in numerical analysis (the courses DN1240 or DN1212 or equivalent) is a prerequisite. We assume that the student has basic knowledge of programming in the languages C or Fortran.

Topics

Linear systems:

- LU-type factorizations and methods
  - sparsity / preservation of sparsity / bandwidth preservation
  - reordering techniques (minimum degree, elimination tree)
  - incomplete factorizations

- Subspace methods: Minres, GMRES, CG, stagnation
- preconditioning: incomplete (LU) factorization, algebraic multigrid
- Software: UMFPACK, ILUPACK

Eigenvalue problems:

- Power iteration / subspace iteration (targets, shift-and-invert)
- Subspace methods:
  - Arnoldi's method (algorithm, choice of target/convergence, orthogonalization, deflation/restarts)
  - Shift-and-invert (inexact solves), change of shift / rational Krylov
  - Jacobi-Davidson
- Software: ARPACK, JADAMILU

Literature

- Chapter 4-5 in [TB] Trefethen, Bau, *Numerical linear algebra*, ISBN:0-89871-361-7. This book is available online to all KTH students.
- The article G. Golub, H. A. van der Vorst, *Eigenvalue computation in the 20th century*, J. Comput. Appl. Math, 2000, 123:35-65, `http://dx.doi.org/10.1016/S0377-0427(00)00413-1`
- The article G. L. G. Sleijpen, H. A. Van der Vorst, *A Jacobi-Davidson iteration method for linear eigenvalue problems*, SIAM Review, 2000, 42(2), 267-293, `http://dx.doi.org/10.1137/S0036144599363084`
- Manuals of the software packages
- Hand-outs covering specific matrix structures

Assessment

The theoretical knowledge will be evaluated by questions to be answered as a part of the lab work. The practical work comprises assignments to the covered aspects of the lecture.

Preliminary schedule

The first lecture is on **Thursday 22/3, 13:15-15:00 in room 1537** Note! New time and day!
The times and dates of other lectures are to be decided.
Deadlines:

- Homework 1: 29/3 (linear systems)
- Homework 2: 18/4 (linear systems)
- Homework 3: 25/4 (eigenvalue problems)
- Homework 4: 6/6 (eigenvalue problems)

Contact

Elias Jarlebring, CSC/NA - Floor 5, Office 4518, eliasj@kth.se