

PHYS 511: Computational Modeling and Simulation - Fall 2017
Assignment #1, due Friday October 27, before class

Getting familiar with Fortran and LAPACK

1. Write a Fortran program that solves a system of linear equations

$$Ax = b, \tag{1}$$

where A is the Hilbert matrix of size $n \times n$. Its elements given by

$$A_{ij} = \frac{1}{i + j - 1},$$

and b is a n -component vector with all elements equal to one, i.e. $b_i = 1$.

The program should take n either as user input from keyboard, or as a command line argument. That means the program *does not know in advance* the value of n .

The output of the program should be the solution vector x saved in a file called `solution.dat`, one component per each line of the file.

In this assignment you do not need to come up with your own algorithm of solving the system of linear equations. Instead, use LAPACK library. You will need to find out which LAPACK subroutine suits your task best. While several subroutines might do the job, you should choose the most optimal one based on the type of the matrix you are dealing with. The usual things to consider when using LAPACK and other numerical linear algebra packages: sparcity (dense or full), symmetry (symmetric/hermitian or not), structure (band matrix or not), type (real or complex), precision (single or double).

2. Use *double precision* in your computations.
3. When the program is written and you made sure it works properly, run it for the case $n = 10$.
4. You can verify the quality of the solution by computing the ratio $\frac{\|Ax-b\|}{\|b\|}$, where $\|\dots\|$ stands for the norm of a vector.
5. *Bonus question:* Did the actual quality meet your expectations? You might recall things such as the condition number of a matrix and how it relates to the expected accuracy of the solution.
6. Put the source file of your program, as well as the solution file for the case $n = 10$, in subdirectory called `as1` in your google-drive directory that is shared with the instructor. You may include other files (e.g. your comments in `comments.txt`) in your submission if you find it necessary.