Computational Physics **Problem Set 6** **Due 2019/11/5**

Your solutions should include your source codes (without *.exe files), results, and discussions. The discussion file as well as the proof in the problem 3 should be prepared with a typesetting system, e.g., LaTeX, Word, etc., and it is converted to a PDF file. All files should be zipped into one gzipped tar file, with a file name containing your student number and the problem set number (e.g., r05202043_ps6.tar.gz). Please send your homework from your NTU email account to twchiu@phys.ntu.edu.tw before 24:00 of the due date.

1. **LU-decomposition with pivoting**

   Write a C or C++ program to perform the *LU*-decomposition of any non-singular matrix (det $A \neq 0$), with the capability of exchanging rows when it encounters zero pivot. Test your program with the following matrix

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 2 \\ 1 & 2 & 1 \end{pmatrix}$$

   Use your code to perform the LU-decomposition of the following matrix (without pivoting).

$$\begin{pmatrix} 1 & 1/2 & 1/3 & 1/4 & 1/5 \\ 1/2 & 1/3 & 1/4 & 1/5 & 1/6 \\ 1/3 & 1/4 & 1/5 & 1/6 & 1/7 \\ 1/4 & 1/5 & 1/6 & 1/7 & 1/8 \\ 1/5 & 1/6 & 1/7 & 1/8 & 1/9 \end{pmatrix}$$

2. **Inverse of a matrix using LU-decomposition**

   Write a C or C++ program to obtain the inverse of any non-singular matrix using the *LU*-decomposition with pivoting. Use your program to find the inverse of the 5 *x* 5 matrix in the last Problem.

3. **Conjugate gradient algorithm**

   Prove the CG algorithm for $A = D^{\dagger}D$ given in the lecture note.

4. **Solve a linear system with conjugate gradient**

   Write a C or C++ program to solve the linear system $C|x\rangle = |b\rangle$. Use your

program to solve the linear system with

$$C = \begin{pmatrix} 1 & 1+0.990*i & 0 & 0.2490 & 0 \\ 0.5000 & 0.3300 & i & 0 & 0.1230 \\ 0 & 2.1230+i & 0.2150 & 0.0131 & 0.0127 \\ 0.2645 & 0 & 0 & 0.0130 & 0 \\ 0 & 0.0010 & 0 & 1.0-8.970*i & 0.0110 \end{pmatrix}, \quad |b\rangle = \begin{pmatrix} 1.001 \\ 1+0.877*i \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

How many iterations does you code take to obtain the solution with the stopping criterion $\varepsilon = 10^{-10}$?