Program directory 'Computational Physics'

Jos Thijssen,
Delft Technical University, The Netherlands
E-mail J.M.Thijssen@tudelft.nl

May 18, 2007

1 Introduction

This note gives a short description of the program directory for the book entitled 'Computational Physics (second edition)' by Jos Thijssen. This book was published by Cambridge University Press. The book contains introductions to various research fields within computational physics, and it is written at the graduate level. It is therefore probably not suitable for an introductory course on the subject.

The book contains descriptions of quite a few programs which can be written by the reader, and in the problems at the end of each chapter, additional programming issues are considered, in addition to theoretical material. The program directory contains the programs described in the chapters as exercises for the reader.

2 Copyright and contacting the author

I would appreciate any comment or correction.
Contact me at J.M.Thijssen@tudelft.nl.

3 Language

The programs are written in Fortran 77 and Fortran 90. I have not everywhere adhered to the f77 standard, but used some extension from the military standard, which are part of most modern f77 compilers, in particular the `DO ... END DO` construct. As a result of this, labels are almost absent in all programs. I also left out the `STOP` and `RETURN` statements in most places.

Most of the programs should work with the gfortran compilers. Please notify me whenever this is not the case. An exception is formed by some of the programs for chapters 11 and 13. For the programs of chapter 11, the

Heisenberg chain is provided in two forms: one for intel's ifort compiler, and one for gfortran. The Heisenberg chain spectrum obtained using symmetry however is given in a program which used some functionality not supported by gfortran – hence this only works for intel. In general intel's compiler is recommended because of its superior performance (it is free for non-commercial use, but difficult to find on intel's web page).

One library is written in C: the XPS graphics library for plotting using X-window graphics. The library is a kind of 'emergency package' which should work with *any* X11 installation as it used the Xlib library and no gui packages of which I always turn out to have the wrong version installed in my linux distribution.

4 The material

The program directory consists of programs, libraries and a utility program. In this section, the various components of the program directory are described.

4.1 Libraries

The libraries should be compiled first. They can be found in the directory '$COMPHY/lib', where '$COMPHY' is the location of the directory. In the directory '$COMPHY/lib' there is a Makefile for creating the libraries. The libraries are 'geneig.a' which contains some convenient interface to the LAPACK routines for solving the generalised eigenvalue problem. The LAPACK and BLAS sources are *not* included: they can be found at `http://www.netlib.org/`. The library libnumer.a contains a simple routine for the numerov integration method for special types of second order differential equations. The library 'libran.a' contains a random generator.

Note that it is best to use the same compiler as used for all your programs in making the library. Mixing intel and gfortran sometimes gives problems with linking.

A separate library is the XPS graphics library (also see above), which contains its own documentation. This contains a collection of graphics routines, written in (old-fashioned K & R) C, for generating X-window graphics or postscript output.

4.2 The programs

The actual Fortran 77 programs can be found in the directories '$COMPHY/ch1'–'$COMPHY/ch15'. Each program contains some information in a comments section at the top. Most importantly, this comments section often says which section of the book the program is described in. Each directory contains furthermore a makefile, which may refer also to some of libraries described above, and perhaps some include files.

4.3 Utilities

The directory '$COMPHY/utils' contains the C-program 'blockdata.c', which does a block average of a file containing correlated statistical data for some real variable. This program can be used to analyse the results from molecular dynamics and Monte Carlo programs. Furthermore, in the directory '$COMPHY/ch8/Ar', there is a file called 'calcres.f', which calculates the potential energy and the quantity $P/(k_{\mathrm{B}}T\rho)$, for a monatomic gas, based on raw data from a simulation in which the Verlet nearest neighbour list has been used.

5 Errata

The book contains errors. Hopefully the second edition contains fewer than the first. I have found just a few tiny errors so far. I will keep a record of all errors found in this document.

- Figure caption 10.3: The drawn line has the form $a(N-1)^{1.5}$, not 0.75 in the exponent.
- Problem 12.5 on page 420:

$$f(r) = \exp\left(\frac{r}{\alpha(1+\beta r)}\right),$$

  i.e. no subscript '12' with r in the denominator.

- The values in columns 8 and 11 of table 12.1 on page 376 have not been calculated correctly. The trend is correct however.
- Just below Eq. (13.11), $x_{ab} = x_a - x_b$. In Eq. (13.20), the third element of the vector should be x_{ba}. In Eq. (13.29), the **C** matrix given should be multiplied by $E/(1-\nu^2)$. And the **B** matrix occurring in (13.38) should read:

$$\frac{1}{2A}\begin{pmatrix} y_b-y_c & 0 & y_c-y_a & 0 & y_a-y_b & \\ 0 & y_c-y_b & 0 & x_a-x_c & 0 & x_b-x_a \\ x_c-x_b & y_b-y_c & x_a-x_c & y_c-y_a & x_b-x_a & y_a-y_b \end{pmatrix}.$$

- In Eq. (14.35), 1/9 is the weight for $i = 1, 3, 5, 7$ and 1/36 for $i = 2, 4, 6, 8$.
- Eq. (15.94) should have $2J$ and not $-2J$ in the exponent.

I would appreciate any comments or corrections to the book or to this program directory. Contact me at `J.M.Thijssen@tudelft.nl`.