1. Computational exercise. Objectives.

The objectives for **Project 1a** are essentially the same as those for Project 1 **except for the following**:

1. **Project 1a** must be completed in a programming environment that is different from that used for Project 1.

2. Only the virial equation of state should be considered. The general form of the virial equation of state is as follows:

$$p = \frac{RT}{V_\mathrm{m}}\left(1 + \sum_{i=1}^{N} \frac{B_{i+1}}{V_\mathrm{m}^{i}}\right) \tag{1}$$

   where coefficients B_i are called *the virial coefficients*. For example, B_2 is called *the second virial coefficient*, B_3 – *the third virial coefficient* etc. Obviously, there is no "*first virial coefficient*", as the first term of this expansion is identical to the ideal gas equation of state:

$$p = \frac{RT}{V_\mathrm{m}} \tag{2}$$

3. Your code must support expansion (1) for any value of N up to, say, 10 !

4. Because equation (1) can contain any number of terms, the input data file format for **Project 1a** is modified as follows:

```
He, virial eos
virial   2
  9.E-01  2.E-05
temp   50.0 K
m^3/mol bar
    4.15723500000000E-02    1.00021078799193E-01
    4.11607425742574E-02    1.01021502604605E-01
    4.07572058823529E-02    1.02021930630615E-01
    4.03615048543689E-02    1.03022362877295E-01
    3.99734134615385E-02    1.04022799344716E-01
    3.95927142857143E-02    1.05023240032949E-01
    3.92191981132075E-02    1.06023684942067E-01
    3.88526635514019E-02    1.07024134072140E-01
    3.84929166666667E-02    1.08024587423241E-01
    3.81397706422018E-02    1.09025044995441E-01
    3.77930454545455E-02    1.10025506788811E-01
```

Line 1: This is a comment line, one can put whatever s(he) wants there, but you need to read this comment and print it out before doing anything else. It is exactly the same as in the Project 1 data files. As before, this line will contain answers to the exercise.

Line 2: This line will always include the "`virial`" keyword followed by the number of terms in expansion (1) to be used.

For example, the "`virial 1`" option requests expansion:

$$p = \frac{RT}{V_\mathrm{m}}\left(1 + \frac{B_2}{V_\mathrm{m}}\right) \tag{3}$$

while the "`virial 3`" command specifies expansion:

$$p = \frac{RT}{V_\mathrm{m}}\left(1 + \frac{B_2}{V_\mathrm{m}} + \frac{B_3}{V_\mathrm{m}^2} + \frac{B_4}{V_\mathrm{m}^3}\right) \tag{4}$$

Note that the keyword "`virial`" can be specified using either lower or upper case letters, or a mixture of those.

Line 3: initial guess for the *N* parameters to be fitted.

The remaining lines have exactly the same meaning as those in the Project 1 data files.

2. Important notes.

1. The fit should be done using the non-linear least squares (NL LSQ) technique outlined in the Project 1 handout. You absolutely can not use built-in NL LSQ or any other optimization options that your software provides (what fun is that anyway?!) in the final production code (which means that you are allowed to use built-in minimization/optimization options for debugging purposes only!).

2. You are allowed to fit the virial equation of state in any of the following forms (you choose which one):

$$pV_\mathrm{m} = \dots \tag{5}$$

$$p = \dots \tag{6}$$

$$\frac{pV_\mathrm{m}}{RT} = \dots \tag{7}$$

whatever is more convenient for you. It is advised that before you perform the fit, you convert the *p*-*V* data to standard SI units (that is, if input data are not in the standard SI units): $\mathrm{m}^3\,\mathrm{mol}^{-1}$ for V_m, and Pa for *p*. Of course, you can do the fit in any units, but then you absolutely must convert your final optimized parameters to the standard SI units,

3. Your code must print out the following information for each cycle:
   a. cycle number,
   b. value of the lambda parameter (λ),
   c. error function value, and
   d. values of the virial coefficients.

4. Once an acceptable minimum has been found, the program must produce
   a. a plot of the fitted virial equation of state with optimized coefficients superimposed on the experimental data points, and
   b. the complete statistics of the fit as described in the "*Suggested implementation of the Levenberg-Marquardt method*" section of the Project 1 handout.

5. Finally, the runtime of the program should be under 1 hour for each dataset.

That's it! Do not forget to submit your program to D2L by the due date/time.