1. *Program Compilation and Run*

Call the DELPHI. Click on FILE, OPEN the PROJECT, and, using the browser, click on vmria.dpr. Press F9 on the keyboard - the program vmria will be compiled, the executable file will be saved in AAA folder and run: a Windows window appears which informs about the output file and has 3 keys: for changing the output file name, for running VMRIA, and for putting comments into the output file. The default name of the output file is mddhhmm.res, where dd is the day, hh - hours, and mm - minutes. The name of the res-file can be changed.

'Go on' clicked, the window with the caption 'VISUAL MRIA +++ 2013' appears on the screen, which then plays the role of a console to run the program and watch its results. The access to the program algorithms is enabled via the main menu.

Once compiled, the program can be called from any folder of the computer.

Each mouse clicking on the keys of the main menu produces event - a request for the execution of a certain program operation - a spectrum input, this or that processing, etc. Each request is replied by a dialog window through which an exchange of data between the user and the program proceeds in a very convenient and straight-forward way.

The hierarchical menu allows the user to browse among the program features and select the optimal strategy of the spectrum analysis.

The key HELP introduces the user into customizing the program: describes the general algorithm, tells how to get started etc. The output information includes also graph-files (in BMP-format), which optionally may be saved at user's request.

To abandon the program click on 'File', then on 'Exit'.

The user may create an ASCII ini-file and have there the most needed data for the program run. Or, if such a file is absent, enter the needed data in a dialog mode - using the corresponding keys. Some sample ini-files for the processing spectra are included into the program package along with the spectra. They are self-commented (an asterisc in the 1st position of the line means comment and is ignored by the program) and may be easily changed and adapted to an arbitrary spectrum.

The analysis results are saved after finishing the main steps of the algorithm (at the user's request) in the output - file (res-file), which will be accessible without the loss of the information only after it is closed, but one can see its current contents by clicking on 'TEST' and 'View res-file'.

2. *Program Test*

VMRIA can be tested in a dialog mode: enter the spectrum, select the needed key on the Main Menu and carry out the corresponding algorithm.

Note: if one does not know what do dialog prompts mean, press the 'OK'- the defaults can allow the program to execute some reasonable action which would inform the user of its full meaning.

For the testing purpose the program package contains several data sets. Also such data can be produced by pressing the key 'TEST' and the keys 'test rietveld', 'test autoindexing', 'test upeak'. They can be then analyzed in the dialog mode.

Here are some standard ini-files.

3. Test the ZrO2 Spectrum

It is a spectrum from a sample which was produced by the IUC commission with a special purpose to test the measuring devices and the programs analyzing their data. So the results of this analysis are known and can be compared with the test results.

The z.ini file contains all the needed information for this test. The data are supplied with comments. Besides it is recommended to read all the helps which are available in VMRIA.

To read z.ini file, click on FILE, then one can proceed step-wise (enter each step of the ini-file) or enter the whole ini-file; then one has to confirm (or reject) the spectrum normalisation and the correction for absorption.

Then click on RIETVELD and on RIETVELD FIT and then in succession on PRE-PARE THE RIETVELD ANALYSIS, MAKE THE RIETVELD ANALYSIS, SHOW THE QUALITY OF RIETVELD ANALYSIS, SAVE THE RESULTS OF RIETVELD ANALYSIS, finally on EXIT AND SHOW GRAPHS.

This is the minimal number of actions needed to perform the Rietveld analysis of the ZrO2 spectrum. In the full dialogue mode the sequence of actions is as follows.

1. Click on FILE, SPECTRUM INPUT and proceed setting binary, 2 bytes per word as file type, and the 5th order for the background; and leaving the default values for all the other quantities.
2. Click on GRAPH, the SPECTRUM. The spectrum graph appears on the screen.
3. Click on MARK,INTERVAL BOUNDS, and on the beginning and and the end of the spectrum interval for the analysis; these points are approximately a=305, b=740. check them clicking on INFO, about the SPECTRUM; if they differ from 305 and 740 one can correct them. Exit from INFO .
4. Click on TRANSFORM, on NORMALIZE. Tick Correction for Absorption,
5. To build the real peak model click on MARK, PEAK MODEL BOUNDS, then on beginning and end points of this peak on the graph; make sure that the bounds are 580-627 and 9 points for the background; smooth the model by selecting MORE SMOOTHING and clicking several times on OK; if the model (the blue graph) is smooth enough, click on QUIT. Reminder: the default peak model is the Gaussian.
6. For the crystallographic information click on ENTER CRYSTAL INFO, then enter the number of phases, phase and atomic information, form the hkl's and click on Exit;
7. Then in succession click on PREPARE, MAKE, SHOW, SAVE Rietveld analysis and on Exit and Show graphs.

To perform just in this test the Powder Match one should similarly repeat the actions, mentioned above, but omitting the use of atomic information.

The estimates of structure factors, obtained by the Powder Match, can be processed using the Fourier synthesis procedure - click on RIETVELD, on FOURIER SYNTESIS, on Take the structure factors from powder match. Two-dimensional z-slices of (X,Y)-Fourier map will be graphed in succession, and finally the 3-dimensional analysis will be performed.

All the operations are logged in the output file mddhhmm, which can be compared with the file z.res'.

4. Test the tetracub Spectrum

The spectrum is obtained from the neutron diffraction on the crystal CuFe2O4, which is a mixture of the tetragonal and cubic phases. The magnetic scattering was neglected. The auxiliary information is contained in the tetracub.ini file. Click on INPUT INI FILE, open the file tetracub.ini, confirm (OK) the normalization and correcting for absorption, click on RIETVELD, then on RIETVELD FIT, then on PREPARE, then on USE AVAILABLE PARAMETER ARRAY, then on OK (key USE AVAILABLE PARAMETER ARRAY being on), then on MAKE RIETVELD ANALYSIS and so on. One can try to use the PseudoVoigt peak model - make the spectrum graph (click on GRAPH SPECTRUM INTERVAL) and make it sure that the single peak (we neglect the contribution of the tetragonal phase here) at the channel 388 is similar to a PseudoVoigtian, or take some other single peak. Then click on PEAKMODELS, on MAKE SPECIAL MODEL, then select the option PseudoVoigt, put 380 and 408 as [a1,a2] of the peak (if it is at 388), click on OK, then set the option 'Go to the fitting', click on OK. If the fitting is success (the green curve statistically repeats the magenta one), set the option 'Exit' and click on OK. Then all the actions are the same as above (click on RIETVELD, etc.).

5. Test the Popa Spectrum

The spectrum has been measured from Zinc oxide Cu K-alpha strained specimen, and was used to determine its unit cell parameters with the help of the Powder match [6]. The popa.ini file contains all the needed information except for the atomic information and parameters. Here a special peak form (Popa peak model) is used.
As usually click on INPUT INI FILE, open the file popa.ini, ignore the warning that the atomic information is absent, click on RIETVELD, then on POWDER MATCH, then on PREPARE. This time the parameters, their bounds and their possible linear dependences are formed by VMRIA, but if they don't provide the fitting convergence, they should be defined by the user.
Next, click on MAKE POWDER MATCH. and so on. Before graphing the initial and the fitted spectra switch on the logarithmic scale: click on SETTING, SCALE MODE, LN, OK. Compare the picture with the file popa_log.bmp.

6. Test the Magnetic Analysis

A spectrum from the specimen $(Nd_{0.772}Tb_{0.228})_{0.5}Sr_{0.5}MnO_3$, measured on a $\lambda = const$ diffractometer, is analyzed.
The crystal is the sum of the 3 phases - 1 atomic phase, and 2 magnetic ones (Mn and Sr are magnetic atoms of the 2nd phase and Nd is the magnetic atom of the 3rd phase).
The sequentce of actions is as above: input the INI-file 'mag.ini', then click on RIETVELD, RIETVELD FIT, PREPARE (using the available parameters), MAKE RIETVELD ANALYSIS etc.

7. Test the Powder Indexing

Enter the auz.ini file. It contains the d-spacings from the Zirconium oxide sample and all the data needed for the powder indexing, including the parameter array. Then click AUTOX, PREPARE and make the preparation using the data from ini-file, i.e. clicking each time OK, then click MAKE POWDER INDEXING etc.

8. Test the Peak Analysis

It is the decomposition of a spectrum into single peaks and the background, and the estimation of their parameters - peak areas, centers and width parameters, and the parameters of the background. The peaks have a very asymmetric form. The method of a real peak model is used.
Click on INPUT INI FILE and input tar.ini file. Then click on UPEAK and in succession on FIND THE PEAKS, PREPARE THE FITTING, MAKE THE FITTING etc.

9. General case.

In the dialog mode (no ini-file available) the user has to enter the spectrum, its variance (if not the Poissonian case) and, if it is a TOF spectrum, enter the corresponding effective spectrum. Then the modes should be set, peak (and background) models should be formed (defaults = the Gaussian for peaks and the polynomial for the background). A TOF spectrum should be normalized and corrected for absorption. The crystallographic information should be read in: about the phases, atoms and hkls; then call the preparation to Rietveld analysis, then the Rietveld fitting, and finally the output of the results: displaying, graphing and saving.
Similarly, the AUTOX and UPEAK procedures are running. To customize the program one can try different modes and algorithms, bearing in mind that the program does not spoil any data and programs so that one can experiment with VMRIA by clicking on any buttons and without taking any precautions.

10. The source codes

- vmria.dpr - the main program, managing the whole organization of the program run.

- vmria00.pas - contains the class definition and data allocation.

- vmria0.pas - implements auxiliary algorithms.

- vmria1.pas - implements calls to the programs responsing to the clicks on the keys of the main menu.

- vmria2.pas - builds forms and basic graphical gadgets - buttons etc.

- vmria3.pas - builds a form for viewing the helps.

- vmria4.pas - reacts on the clicks on the graph points.

- vspectr.pas - implements the TSPECTRUM class.

- vpmodel.pas - implements the TPEAKMODEL class.

- vpeaksr.pas - implements the TPEAKSEARCH class.

- vgfit.pas - implements the TPARAMETER class - for the least square fitting.

- vmriasim.pas - implements the data simulation.

- vstdcons.pas - builds the most important graphical gadgets.

- vdata.pas - contains test spectra.

- vmriafl.pas - implements responses to clicking on KEY.

- vmriasg.pas - implements responses to clicking on SETTINGS, GRAPH and PEAK-MODELS.

- vmriatr.pas - implements responses to clicking on TRANSFORM.

- vmriartv.pas - implements responses to clicking on RIETVELD.

- vmriainf.pas - implements responses to clicking on INFO.

- vmriauto.pas - implements responses to clicking on AUTOX.

- vmriaup.pas - implements responses to clicking on UPEAK.

- vmriahlp.pas - implements responses to clicking on HELP.

- vtest.pas - implements responses to clicking on TEST.

vzlocom.pas, varfun.pas - contain general purpose procedures.
vmriahkl.pas, vmriahkl.pas - provide for the input and the forming of crystallographic information for RITVELD and AUTOX algorithms.
vmriaini.pas - implements the processing of INI-data files.
vmriarit.pas - arithmetic procedure for the RIETVELD least squares fitting.
vmriarix.pas - arithmetic procedure for the AUTOX least squares fitting.
vspeva1.pas - not yet implemented.
vmria1.dfm, vmria2.dfm, vmria3.dfm, vmria4.dfm - form descriptions.
vmria.cfg, vmria.res, vmria.dof - DELPHI auxiliary files.