

# Automation of ANAELU 2D-XRD texture analysis refinement through Intelligent Computing

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## ABSTRACT

The present work consists on the implementation of the **Nelder-Mead** algorithm for the automation of the model-to-experiment fitting in two-dimensional diffraction texture research

## BACKGROUND

Recently developed x-ray 2D detectors generate the demand for fast and reliable tools for 2D-XRD patterns interpretation. The CIMAV Crystallography Group is active in this field, having introduced the novel software package ANAELU. This Rietveld-style program allows the characterization of polycrystal structure, particularly texture evaluation, by means of 2D-XRD modeling and fitting to experimental data. Previous versions of ANAELU worked accurately, but, due to the manual character of the parameters optimization, its application represents a slow process. By means of the present work the ANAELU group enters a renovation process for the program, introducing the automatic-fitting option for various parameters of the model pattern.

## METHOD

The technique selected for the parameters optimization is the Nelder-Mead(NM) simplex algorithmic method. This algorithm was adapted through a python code and connected with the ANAELU GUI. The whole package has been coded in both Python and Fortran.

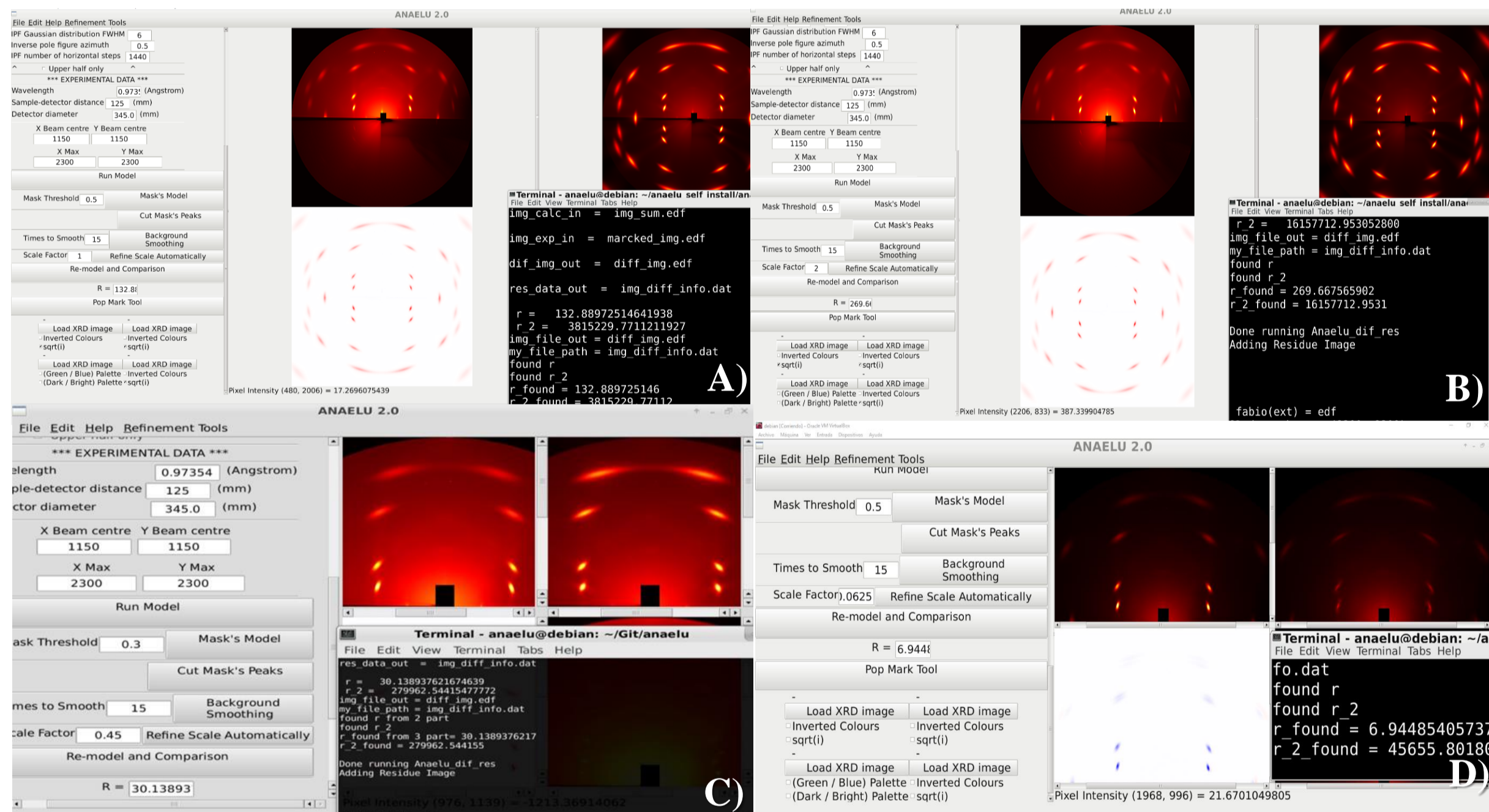


Figure 1. A) Zeroth Cycle, B) First Cycle, C) Third Cycle, D) Fifth Cycle.

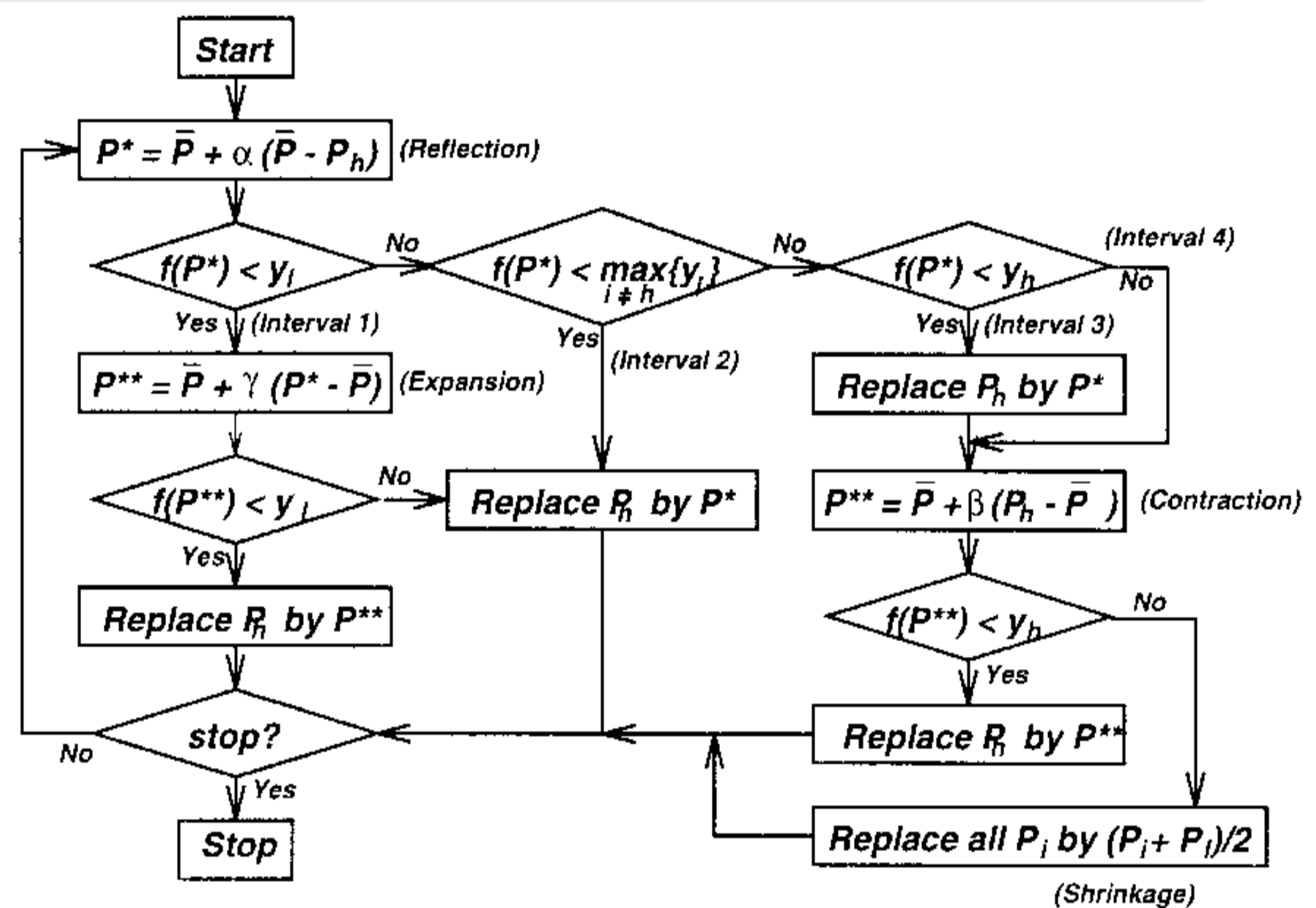


Figure 2. Flowchart for downhill simplex search.

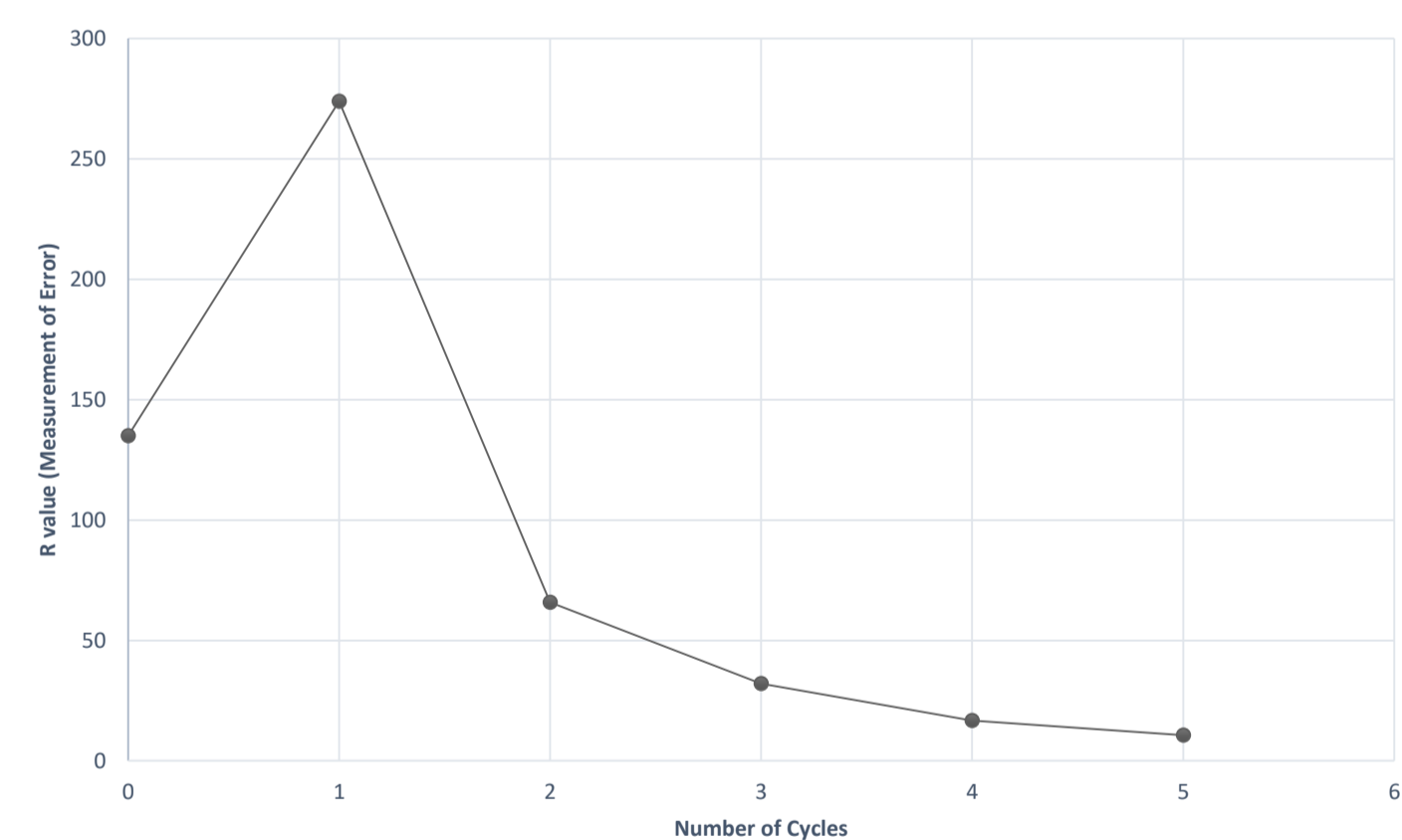


Figure 3. Algorithm Performance in ANAELU

## CONCLUSIONS

- The implementation of the Nelder-Mead algorithm in ANAELU showed to have a positive impact during the refinement process.
- The automatic fitting process runs fast and stably
- By means of the current contribution, ANAELU gets significantly close to becoming the first 2D Rietveld –oriented texture analysis program

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