

# What's new in **SIMPAT** ?

(T.R/CDIFX/2008-2013)

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Oct. 2013

- if `NPROF=7` is specified, the input reflection profiles are characterized by the full widths at half maximum of the gaussian ( $H_G$ ) and lorentzian ( $H_L$ ) parts of a Voigt function. Thompson-Cox-Hasting formula will then be used to calculate the *FWHM* and  $\eta$  parameters of the equivalent Pseudo-Voigt function

April 2009

- background can be described through background points contained in a background file with the help of the `BACK_FILE` keyword. In such a case, background value is calculated by linear interpolation of background values.

ex : `BACK_FILE = my_background.xy`

January 2009

- background simulated by a polynomial function (max. order = 6)

`back = b0 + b1.X + b2.X**2 + ... + b5.X**5`

- background is stored in `simpat.bac` file (XY format)
- background file is included in the `simpat.buf` file

December 2008

- command line arguments :
  - `PLOT` : plot of whole simulated pattern
  - `PLOT_ALL` : plot of whole simulated pattern and individual reflections patterns