LeBail Fit

Mantid Algorithm/CurveFitting

Problem To Solve

- Brief: Fit multiple peaks from model to powder diffraction data;
- Parameters to fit
  - Lattice constant: a, b, c, alpha, beta, gamma
  - Backgrounds
  - Zero shift
    - For POWGEN: Zero, Zerot
  - Powder diffractometer instrument geometry:
    - For POWGEN: Dtt1, Dtt2, Dtt1t, Dtt2t
  - Peak profile
    - For POWGEN: : alph0, alph1, beta0, … …
- Workflow from parameters to diffraction pattern
  - Read input
    - Parameters to fit
    - Non-annihilated reflections (Miller indices)
  - Calculate background
  - Calculate peaks' intensities
    - From input peak parameters and observed diffraction pattern
  - Calculate peaks
    - Each peak's profile parameters are calculated from d-spacing, dtt1, dtt2, alph0, alph1, beta1 and etc.

LeBail Function – From Inputs To Peaks

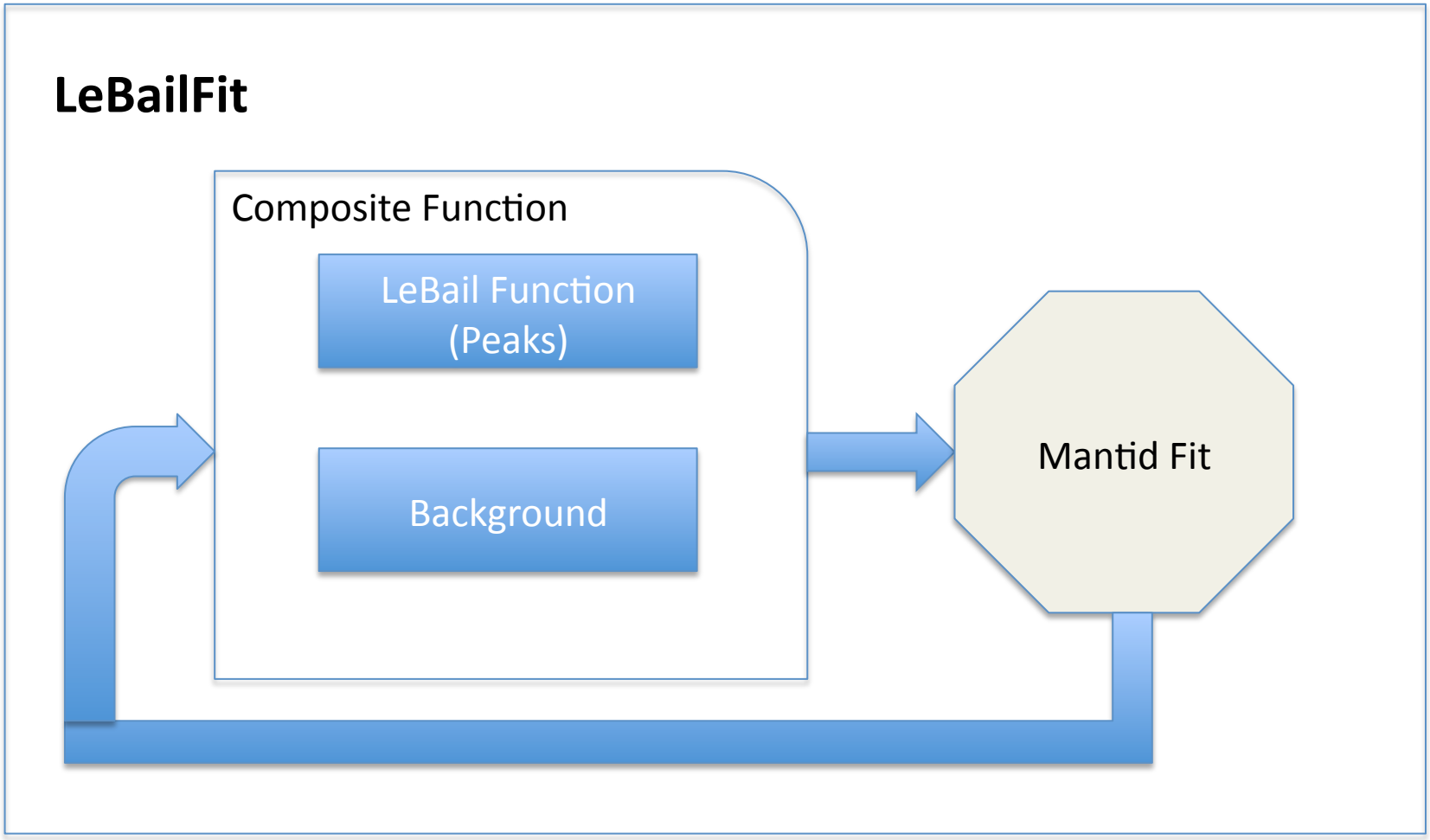
- For each input peak (Miller Index)
  1. Calculate its peak position in d-spacing
     - Lattice constants (a, b, c, alpha, beta, gamma)
  2. Calculate its peak position in TOF
     1. Instrument geometry (Dtt1, Dtt2, Dtt1t, Dtt2t)
  3. Calculate peak profile parameters as function of d-spacing
     1. alph0, alph1, alph0t, alph1t
     2. beta0, beta1, beta0t, beta1t
     3. Sig0, Sig1, Sig 2
     4. Gam0, Gam1, Gam2
  4. Calculate peak profile function

Notes

- Math: The formulas are listed in the PDF file

- Name: In Mantid, the curving fitting function is name *LeBailFunction*, which may not be general enough. Because it uses the formalism of thermal neutron peak profile (Fullprof peak profile #10).

Code Structure



LeBail Function