

FitAllB version 1.0.0

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Contents

1	Introduction	3
2	Mathematical equations	3
2.1	Basic equations	3
2.2	Strain tensor definition	4
2.2.1	Rotating the strain tensor	4
2.3	Error estimation	5
3	Algorithm	6
3.1	Global parameter refinements	6
3.2	Grain parameter refinements	8
3.2.1	Far-field detector only	8
3.2.2	Near- and far-field data	8
4	Input	11
4.1	Example of FitAllB input files	15
4.1.1	Grain parameter fitting, far-field detector only	15
4.1.2	Grain parameter fitting, near- and far-field data	16
4.1.3	Global parameter fitting, far-field only	17
5	Output	18
6	Outlier rejection	20
6.1	Based on internal angles	20
6.2	Based on intensities	20
6.3	Based on residuals	21

6.3.1	Based on residuals, robust	21
6.3.2	Based on average residuals	21
6.4	Peaks assigned to multiple grains	21
6.5	Merging of grains	22
7	Installation and execution	22
7.1	Required packages	22
7.2	Execution	23
7.3	Provided test examples	23
7.4	Contact	24

1 Introduction

The FitAllB program, a part of the FABLE suite of programs for analysis of 3DXRD data (<http://fable.wiki.sourceforge.net/>), is tailored to do centre-of-mass (COM) refinements of grain orientations, positions and strain tensors from far-field images of a polycrystalline material. The name FitAllB originates because the routine fits all \mathbf{B}_i (1), the grain specific reciprocal space metric which contains information about the strain state of the grain.

The aim is to be able to handle several hundred illuminated grains and obtain the strain tensors to an accuracy of 10^{-4} . The strain tensors are output both in the Cartesian grain coordinate system relative to the grain orientation and in the sample system for overall comparisons, and if the components of the stiffness tensor \mathbf{C} are provided, the stress tensors in the same two representations will also be output. FitAllB includes an error estimation routine to give standard deviations of all refined parameters. Finally the relative volumes of the grains are refined, so in principle a 3D orientation and stress/strain map of the polycrystal can be obtained using tessellation.

2 Mathematical equations

2.1 Basic equations

The refinements performed within FitAllB are done using the Variable Metric Minimisation routine of MINUIT [James, 1972] to minimise the following χ^2 -function:

$$FCN = \sum_{i,j(i)} \left(\mathbf{\Gamma}_{ij}^{-1} \bar{\mathbf{G}}_{ij} - \frac{\lambda}{2\pi} \mathbf{U}_i \mathbf{B}_i \bar{\mathbf{G}}_{hkl,ij} \right)^T \mathbf{V}_{ij}^{-1} \left(\mathbf{\Gamma}_{ij}^{-1} \bar{\mathbf{G}}_{ij} - \frac{\lambda}{2\pi} \mathbf{U}_i \mathbf{B}_i \bar{\mathbf{G}}_{hkl,ij} \right) \quad (1)$$

i.e. the deviation from the ideal diffraction equation. The sum is taken over i grains with $j(i)$ reflections in the i 'th grain. $\bar{\mathbf{G}}_{hkl,ij}$ is the assigned hkl of the reflection, \mathbf{B}_i is the grain specific reciprocal space metric, which is connected to the strain tensor as described in Section 2.2, and \mathbf{U}_i gives the orientation of the grain in the rotated system. $\mathbf{\Gamma}_{ij} = \mathbf{\Phi}_x \mathbf{\Phi}_y \mathbf{\Omega}(\omega_{ij})$ relates the rotated system to the laboratory system, \mathbf{V}_{ij} is the covariance matrix of $\mathbf{\Gamma}_{ij}^{-1} \bar{\mathbf{G}}_{ij}$, and the unrotated scatter vector in reciprocal space, $\bar{\mathbf{G}}_{ij}$, can be expressed in terms of direct space quantities:

$$\bar{\mathbf{G}}_{ij} = \left[\frac{\bar{d}_{ij}}{|\bar{d}_{ij}|} - \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right], \quad (2)$$

where:

$$\bar{d}_{ij} = \mathbf{R} \begin{pmatrix} 0 \\ (y_{det,ij} - y_{det,0})p_y \\ (z_{det,ij} - z_{det,0})p_z \end{pmatrix} + \begin{pmatrix} L \\ 0 \\ 0 \end{pmatrix} - \mathbf{\Gamma}_{ij} \begin{pmatrix} x_{0,i} \\ y_{0,i} \\ z_{0,i} \end{pmatrix}. \quad (3)$$

Refineable are 12 parameters per grain (3 positional $(x_{0,i}, y_{0,i}, z_{0,i})$, 3 rotational (\mathbf{U}_i) and 6 strain (\mathbf{B}_i)) and the 10 global parameters: tilt $(\mathbf{R}, 3 \text{ parameters})$, sample-to-detector distance (L) , pixels sizes $(p_y \text{ and } p_z)$, beam centre on detector $(y_{det,0}, z_{det,0})$, and the tilt of the ω -axis around x and y $(\Phi_x \text{ and } \Phi_y)$.

The measured quantities are ω_{ij} , $y_{det,ij}$ and $z_{det,ij}$, thus 3 observables per reflection.

2.2 Strain tensor definition

The grain specific reciprocal space metric of (1) relating reciprocal space to the Cartesian grain system is defined from the reciprocal lattice constants as [Poulsen, 2004]:

$$\mathbf{B}_i = \begin{pmatrix} a_i^* & b_i^* \cos(\gamma_i^*) & c^* \cos(\beta_i^*) \\ 0 & b_i^* \sin(\gamma_i^*) & -c_i^* \sin(\beta_i^*) \cos(\alpha_i) \\ 0 & 0 & c_i^* \sin(\beta_i^*) \sin(\alpha_i) \end{pmatrix} \quad (4)$$

and its direct space counterpart relating any direct space coordinate system to the Cartesian grain system is given as:

$$\mathbf{A}_i = \begin{pmatrix} a_i & b_i \cos(\gamma_i) & c_i \cos(\beta_i) \\ 0 & b_i \sin(\gamma_i) & -c_i \sin(\beta_i) \cos(\alpha_i^*) \\ 0 & 0 & c_i \sin(\beta_i) \sin(\alpha_i^*) \end{pmatrix}. \quad (5)$$

Seing that the elastic strain tensor gives the perturbation of the local lattice in real space we define it as:

$$\epsilon_i = \frac{1}{2} (\mathbf{A}_i \mathbf{A}_0^{-1} + (\mathbf{A}_i \mathbf{A}_0^{-1})^T) - \mathbf{I}, \quad (6)$$

where \mathbf{A}_0 is (5) for the undeformed lattice and \mathbf{I} is the identity matrix. From this it is clear that there is a one-to-one correspondence between the strain tensor components and the elements of \mathbf{B}_i if the undeformed lattice constants are known.

The strain tensor as defined in (6) is sometimes termed the linear Lagrangian strain tensor [Schlenker et al., 1978].

2.2.1 Rotating the strain tensor

The strain tensor as defined above relates to the Cartesian grain system which is rotated by \mathbf{U}_i relative to the sample system. Below is sketched how the different coordinate systems are related:

$$\begin{array}{ccc}
\text{undeformed} & \mathbf{U}_{i,0} & \text{undeformed} \\
\text{sample} & \longleftrightarrow & \text{Cartesian grain} \\
\text{coordinate system} & \mathbf{U}_{i,0}^T & \text{coordinate system}
\end{array}$$

$$\mathbf{A}_0^{-1} \downarrow \uparrow \mathbf{A}_0$$

$$\begin{array}{c}
\text{direct space reference} \\
\text{coordinate system}
\end{array} \tag{7}$$

$$\mathbf{A}_i \downarrow \uparrow \mathbf{A}_i^{-1}$$

$$\begin{array}{ccc}
\text{deformed} & \mathbf{U}_i & \text{deformed} \\
\text{sample} & \longleftrightarrow & \text{Cartesian grain} \\
\text{coordinate system} & \mathbf{U}_i^T & \text{coordinate system}
\end{array}$$

From this it can be derived that if ϵ_i is the strain in the Cartesian grain coordinate system describing the difference between the undeformed and deformed crystal lattices, then:

$$\epsilon_i^{sample} = \mathbf{U}_i \epsilon_i \mathbf{U}_i^T \tag{8}$$

is the strain tensor in the sample coordinate system. Here it has been assumed that $\mathbf{U}_i = \mathbf{U}_{i,0}$ since only \mathbf{U}_i and not $\mathbf{U}_{i,0}$ can be obtained from the diffraction experiment. In the case of elastic deformation this is a good approximation, but it does not hold in the plastic deformation regime where grain rotations are non-negligible.

2.3 Error estimation

The covariance matrix of $\mathbf{\Gamma}_{ij}^{-1} \overline{G}_{ij}$, \mathbf{V}_{ij} , is assumed to be diagonal (thus no covariance) and equivalent for all reflections corresponding to a specific grain. Assuming that the experimental error on ω_{ij} is significantly larger than the error on the detector coordinates $y_{det,ij}$ and $z_{det,ij}$ and remembering that:

$$\mathbf{\Gamma}_{ij}^{-1} \approx \begin{pmatrix} \cos(\omega_{ij}) & \sin(\omega_{ij}) & 0 \\ -\sin(\omega_{ij}) & \cos(\omega_{ij}) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{9}$$

we must have $\mathbf{V}_{ij}^{11} \approx \mathbf{V}_{ij}^{22} > \mathbf{V}_{ij}^{33}$. This relative weighting of the errors in x , y and z is taken into account by setting $\mathbf{V}_{ij}^{11} = \mathbf{V}_{ij}^{22} = 4 \cdot 10^{-8}$ and $\mathbf{V}_{ij}^{33} = 10^{-8}$. If these error estimates are correct the contribution from grain i to (1) must be equal to the number of observation minus the number of refined parameters [Eadie et al., 1971],

thus in most cases $3 \cdot j(i) - 12$. In case the contribution from grain i to (1) differs from the predicted value, the estimated experimental errors are scaled to make the observed contribution equal to the prediction. The errors on the refined parameters are then calculated by the MINUIT [James, 1972] to be the change in each parameter causing the value of (1) to increase by 1.

3 Algorithm

The FitAllB program package is written in python and contains 3 different scripts which basically run the same minimisation in different preset modes. The reason for this is that grain and global parameters cannot be refined simultaneously because of correlations, but in order to obtain accurate grain resolved strain tensors it is of the utmost importance that the global parameters relating to the experimental setup are well calibrated.

fitglobalgrain.py is used to refine the global parameters using one grain at the time. The final values and estimated errors are then obtained as the average and spread over all grains.

fitglobal.py is used to refine the global parameters using all grains in one go. This procedure is more time consuming, but less affected by outlier grains.

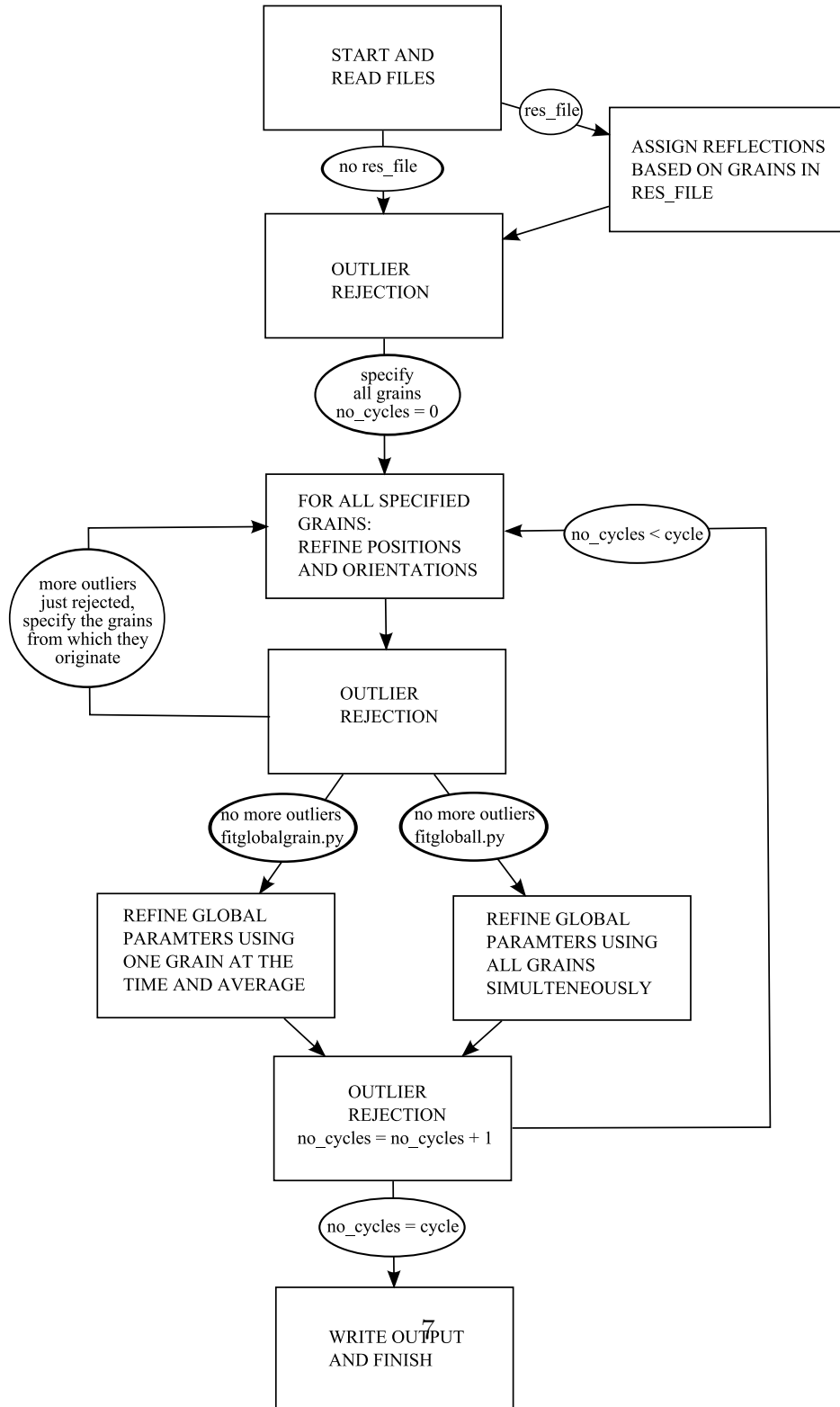
fitallb.py is the main script for refining COM positions, orientation and strain tensors after having calibrated the global parameters. Only grain specific parameters are refined. If near-field diffraction data are available these are initially used to fit the grain positions, which are then kept fixed in the subsequent far-field refinement of orientations and strains.

3.1 Global parameter refinements

The calibration or refinement of global parameters must be performed using an undeformed polycrystalline sample. A good start guess on both the global parameters (ImageD11) and grain orientations and positions (GrainSpotter) is a prerequisite. The refinement is then carried out by alternately refining the global parameters and the grain parameters (positions and orientations) for a preset number of cycles to minimise correlations. An overview of the refinement procedure is given in Figure 1.

When fitting the global parameters the tilt of the sample stage corresponding to a rotation around the beam (in ImageD11 called χ , in FitAllB called w_x , c.f. Table 3) is kept fixed as this correlates with the detector tilt component corresponding to a rotation around the same axis (ImageD11: tilt_x , FitAllB: tx). Furthermore the beam centre in the z -direction (ImageD11: z_center , FitAllB: cz) is kept fixed as this correlates with the grain positions along z . After every cycle the refined global

Figure 1: Flowchart of global parameter refinements using an undeformed polycrystalline sample. Results from position and orientation step saved in stem_rotpos#.gff, from globals step in stem_globals#_fab.par, where # = no_cycle



parameters are output in an ImageD11 format detector.par file. After the global parameter calibration this detector.par file can be used as input to the fitallb.py grain refinements so accurate grain parameters can be obtained.

3.2 Grain parameter refinements

3.2.1 Far-field detector only

An overview of the grain parameter refinement procedure using only far-field data is given in Figure 2. Note that there are two different ways to assign diffraction peaks to the refined grains: 1) Using the assignment given in the grainspotter.log, or 2) Reading the initial grain parameters from a .gff (Section 5) and using these to do a forward projection onto the far-field detector to harvest diffraction spots. It may happen that the number of assigned peak is higher than actually possible because very loose cuts are being used, but these falsely assigned peaks will eventually be removed as outliers. In the long run, perhaps it should be possible for the user to supply the cuts?

3.2.2 Near- and far-field data

An overview of the grain parameter refinement procedure using both near- and far-field data is given in Figure 3. Here the grain positions and orientations in the grainspotter.log of the far-field data is used to do a forward projection onto the near-field detector to do the assignment of reflections. The comments given in the previous section regarding forward projection also holds here.

Figure 2: Flowchart of fitallb.py for refinements using only far-field data. Results from first refinement step saved in stem_grain.gff, subsequent refinements in stem_final.gff

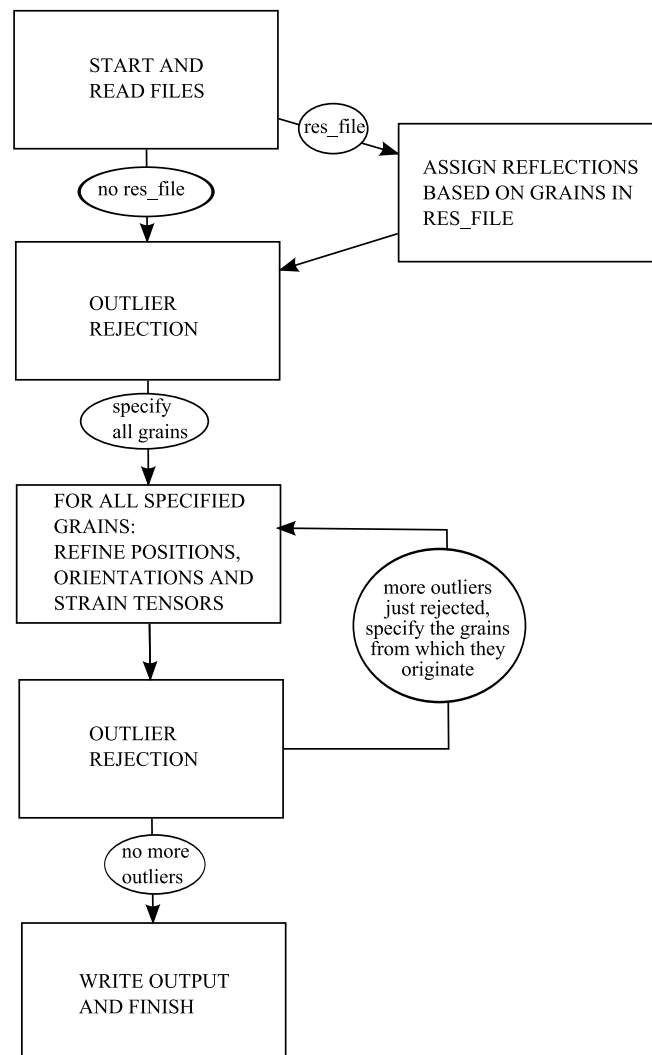
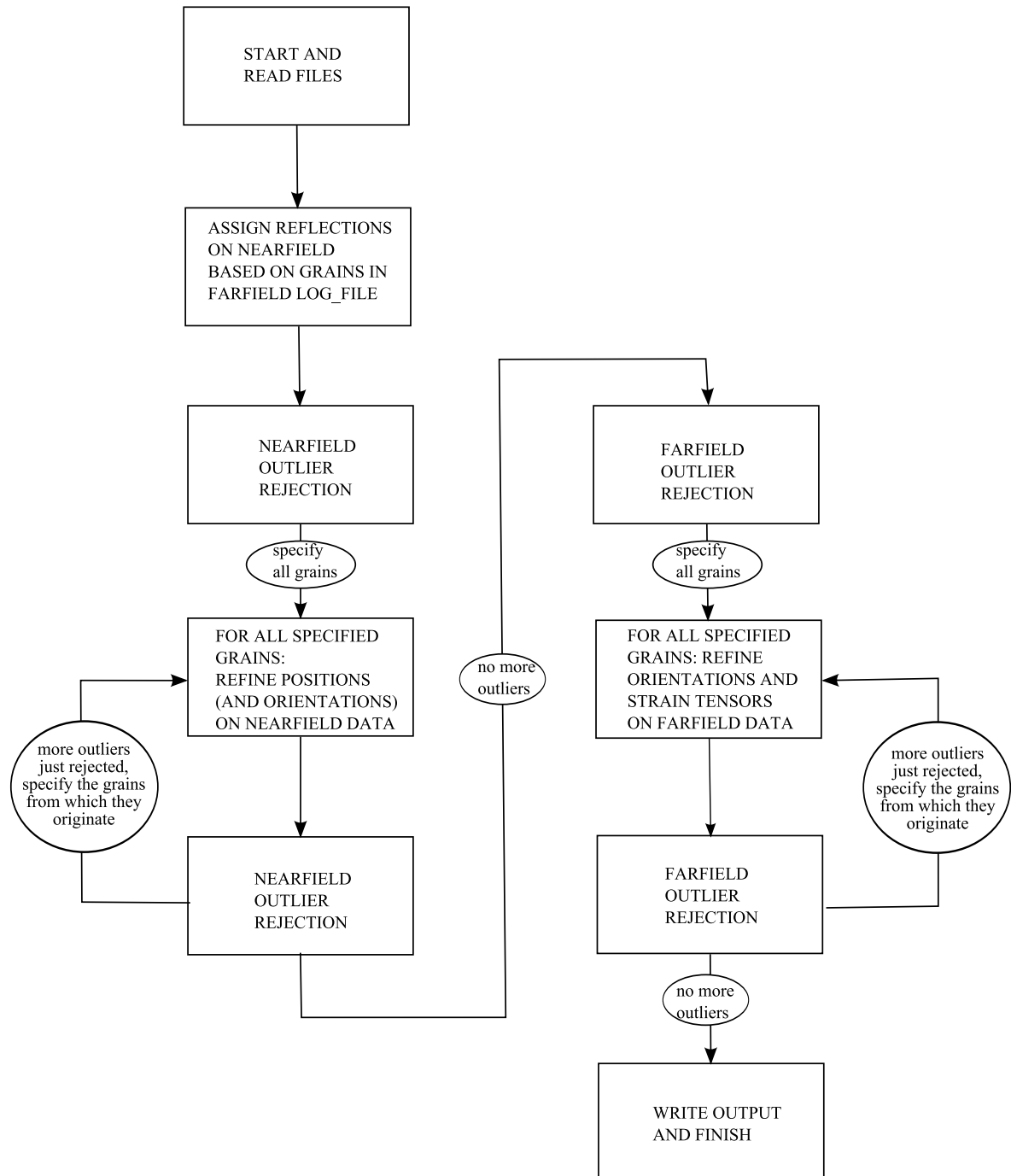


Figure 3: Flowchart of fitallb.py for refinements using both near- and far-field data. Results from near-field step saved in stem_near_rotpos.gff, from first far-field step in stem_grain.gff and subsequent steps in stem_final.gff



4 Input

The main input file for `fitallb.py/fitglobalgrain.py/fitglobal.py` is an ascii file with any name containing a number of mandatory and optional commands with a given syntax. These commands contain information about all the remaining files to be read (Table 1), the experimental setup (Table 2), which parameters to fit and tolerances to use (Table 3), and what kind of outlier rejection to perform (Table 4). The commands can be given in any order, the optional ones can be left out if the default values should be used, and comments can be inserted in the input file by the use of `#` (see input examples in Section 4.1)

Table 1: List of input file commands.

Mandatory commands are given in boldface.

command	usage
log_file	Name of the log file from GrainSpotter to be read Contains number of grains, and for each grain: \mathbf{U} , (x, y, z) , and for all assigned peaks: $h, k, l, 2\theta, \eta, \omega, \text{peak_id}$
flt_file	Name of the filtered peaks file from peaksearch to be read Contains the filtered peaks, for each peak: $\text{peak_id}, y_{det}, z_{det}, \omega, I$
par_file	Name of the detector.par file from ImageD11 to be read Contains the experimental parameters: unstrained unit cell, wavelength, tilt, sample-to-detector distance etc.
near_flt_file	Name of the nearfield filtered peaks file
near_par_file	Name of the nearfield detector.par file
structure_file	(possible formats .cif or .pdb) Contains information about the crystal structure that is used for outlier rejection based on intensities (Section 6.2)
res_file	Read starting values of grain parameters from this .gff (grain file format). If used the peaks assigned to each grain in the grainspotter.log are replaced by matches made by fitallb based on the grain parameters in res_file.

Table 2: List of experimental setup and sample commands.

Mandatory commands are given in boldface.

title	Anything to specify the refinement NB! Remember to use quotation marks: 'my very own refinement specifying title'
w_step	Step size in ω
w_limit	Limits of the ω -intervals [deg] collected, e.g. -150 -30 30 150 min and max for every interval must be given, order irrelevant, thus 150 30 -150 -30 is equivalent to the above. If the data are collected as only one interval, w_limit can be omitted as the limits can be determined from the filtered peaks file. Used to reject peaks on the edges of the ω -intervals.
bg near_bg	Average background levels on far- and nearfield detectors. Used to reject overflown peaks, i.e. peaks with a maximum intensity above $2^{16} - \text{bg}$. Defaults: bg 1000, near_bg 100
dety_size detz_size near_dety_size near_detz_size	Farfield detector size along y and z in pixels default values are 2048 and 2048. Nearfield detector size along y and z in pixels default values are 1536 (y) and 1024 (z). Used to reject peaks close to the edges of the detector and to convert to the ImageD11 beam centre convention in case of a flipped detector, so it is important to check whether the defaults are correct.
crystal_system	Used for setting up stiffness tensor, allowed possibilities: isotropic, cubic, hexagonal, trigonal_high, trigonal_low, tetragonal_high, tetragonal_low, orthorhombic, monoclinic, triclinic. This information is also important for converting the orientation into the fundamental zone, therefore it is mandatory. isotropic is used for cubic with isotropic elasticity. trigonal_high: 32, 3m, $\bar{3}m$ trigonal_low: 3, $\bar{3}$ tetragonal_high: 422, 4mm, $\bar{4}2m$, 4/mmm tetragonal_low: 4, $\bar{4}$, 4/m
stress	convert strain to stress, (1=yes/0=no), default: 0
c11, c12, etc.	Stiffness constants for strain to stress conversion (stress 1). The program will stop if the supplied c's are not enough to fulfil the requirements of the crystal system. A list of required c's for each crystal_system is given on the wiki: http://fable.wiki.sourceforge.net/FitAllB
beampol_factor	Beam polarisation factor, 1: fully plane polarised (default), 0: unpolarised
beampol_direct	Direction of the normal to the plane of the primary beam polarisation with respect to the sample rotation axis [deg], e.g. if the ω -axis is parallel to the z-axis the value is 0 (default), and if the ω -axis is along the y-axis it is 90.

Table 3: Fit options: Parameters and tolerances. NB! The global parameters can only be refined when calling fitglobalgrain.py/fitgloball.py

command	usage
w	Fit omega stage tilt parameter wy (1=yes/0=no), default: 0
tilt	Fit detector tilt parameters tx, ty, tz (1=yes/0=no), default: 0
pixel	Fit pixel size py and pz (1=yes/0=no), default: 0
center	Fit beam centre on detector along y, cy (1=yes/0=no), default: 0
L	Fit sample-to-detector distance (1=yes/0=no), default: 0
xyz	Fit positions on far-field (1=yes/0=no), default: 1
rod	Fit orientations and thus Rodrigues vectors on far-field (1=yes/0=no), default: 1
eps	Fit strain tensors on far-field (1=yes/0=no), default: 1
near_xyz	Fit positions on near-field (1=yes/0=no), default: 0 NB! If near-field data are read (near_fit_file and near_par_file) it is important to set near_xyz 1, fit positions on near-field, and xyz 0, do not fit positions on far-field, because otherwise the accurate positions refined on the near-field detector will be overwritten in the far-field refinement step, c.f. Figure 2.
near_rod	Fit orientations and thus Rodrigues vectors on near-field (1=yes/0=no), default: 0
near_eps	Fit strain tensors on near-field (0=no only option)
tol_step	where step can be rotpos, grain or global, c.f. algorithm flowcharts. Fit tolerance used in the corresponding refinement step. Defaults are: tol_rotpos = tol_global = 1e-2 and tol_grain = 1e-3. Note that the program sets tol_final = tol_grain*0.1. The refinement is considered converged when the estimated distance to the minimum is less than 10^{-3} times the specified tolerance.
cycle near_cycle	Number of cycles for fitglobalgrain.py/fitgloball.py, default=20

Table 4: Outlier rejection commands. *All commands except skip can be used in a near_ option to specify different outlier rejection limits for the near-field data.

command	usage
rej_ia	Outlier rejection limit in degrees for gvector misorientation, Section 6.1. All peaks with misorientations larger than this are rejected. Default: 0.2.
rej_vol	Outlier limit for volume/intensity based rejection, Section 6.2. NB! Requires a valid structure_file command. Default: 5.
rej_resmedian	Outlier limit for robust residual based rejection, Section 6.3.1. Default: 5.
rej_resmean	Outlier rejection limit in terms of average peak contributions, Section 6.3.2. Default: 10.
rej_multi	Remove peaks assigned to more than one grain (1=yes/0=no), Section 6.4. If yes (default) the peak is removed from the grain where the fit (in terms of residual and volume/intensity) is poorest.
overlap	Criteria for merging grains, Section 6.5. Grain with a larger fraction of overlapping grains than specified are merged. Default: 1., i.e. no merging.
min_refl	If the number of reflection assigned to a grain drops below the specified value the grain is skipped in subsequent refinement steps. Defaults: min_refl 9, near_min_refl 3.
skip*	Used to rule out specific grains from the GrainSpotter log file that for some reason or another are known to be poor.

4.1 Example of FitAllB input files

4.1.1 Grain parameter fitting, far-field detector only

```

title 'IF steel, experimental data, undeformed layer 50'
##### Mandatory input files, farfield strain fitting
log_file S1_e0_050_grainspotter.0.35.log
flt_file S1_e0_050.flt
par_file frelon_fitted_july08.par
##### Additional file to be read for volume based outlier rejection
structure_file IF_steel.cif
##### Mandatory experimental parameters
dety_size 2048      # detector dimension [pixels]
detz_size 2048      # detector dimension [pixels]
w_step 0.5          # step size in omega [deg]
w_limit -22.5 22.5 67.5 112.5  # limits of omega intervals [deg]
crystal_system cubic
##### on/off possibilities for fitting
# Global parameters, do not fit.
# This is the default and only option, so no need to specify
# Grain parameters, fit all
rod 1               # Fit orientations and thus Rodrigues vectors (1=yes/0=no)
xyz 1               # Fit positions (1=yes/0=no)
eps 1               # Fit strain tensors (1=yes/0=no)
##### Outlier rejection information
rej_ia 0.2          # Outlier limit in deg for gvector misorientations
rej_vol 5           # Outlier limit for volume/intensity based rejection
rej_resmedian 10    # Outlier limit for robust residual based rejection
rej_resmean 5       # Outlier rejection limit in terms of average peak contribution
rej_multi 1         # Reject peaks assigned to more than one grain
min_refl 36         # Require 36 assigned reflections for good grain
overlap 1           # grain overlap tolerance
skip 31 45          # skip grains 31 and 45 in the GrainSpotter log_file
##### Tolerances
tol_grain 1e-3
##### Parameters for strain-to-stress conversion
stress 1
c11 23.7e10
c12 14.1e10
c44 11.6e10

```

4.1.2 Grain parameter fitting, near- and far-field data

```

title '10 grains of IF steel, 2 detectors'
##### Mandatory input files, farfield strain fitting
log_file if100_t50_10.log
flt_file if100_t50.flt
par_file if100.par
##### Additional files for nearfield position fitting
near_flt_file if100_near_t50.flt
near_par_file if100_near.par
##### Additional file to be read for volume based outlier rejection
structure_file IF_steel.cif
##### Mandatory experimental parameters
w_step 0.5 # step size in omega [deg]
w_limit -22.5 22.5 67.5 112.5 # limits of omega intervals [deg]
dety_size 2048 # farfield detector dimension [pixels]
detz_size 2048 # farfield detector dimension [pixels]
near_dety_size 1536 # nearfield detector dimension [pixels]
near_detz_size 1024 # nearfield detector dimension [pixels]
crystal_system cubic
##### Parameters for strain-to-stress conversion
stress 1
c11 23.7e10
c12 14.1e10
c44 11.6e10
##### Outlier rejection information
# Use default rej_ for both detectors, thus no need to specify values in input
min_refl 36 # Require 36 assigned reflections for good grain on farfield
near_min_refl 30 # Require 30 assigned reflections for good grain on nearfield
##### on/off possibilities for fitting
# Global parameters, do not fit
# This is the default and only option, so no need to specify
# Grain parameters, farfield
xyz 0 # Do not fit positions on farfield
rod 1 # Fit orientations and thus Rodrigues vectors on farfield
eps 1 # Fit strain tensors on farfield
# Grain parameters, nearfield
near_xyz 1 # Fit positions on nearfield
near_rod 0 # Do not fit orientations and thus Rodrigues vectors on nearfield
near_eps 0 # Do not fit strain tensors on nearfield
##### Tolerances
tol_grain 1e-3
tol_rotpos 1e-2

```


4.1.3 Global parameter fitting, far-field only

```
title 'fitglobal1 5 undeformed grains of IF steel, 20 cycles'
##### Mandatory input files
log_file if100_globals_wedge_5.log
flt_file if100_globals_wedge.flt
par_file if100_globals_wedge.par
##### Additional file to be read for volume based outlier rejection
structure_file IF_steel.cif
##### Mandatory experimental parameters
dety_size 2048      # detector dimension [pixels]
detz_size 2048      # detector dimension [pixels]
w_step 0.5          # step size in omega [deg]
w_limit -22.5 22.5 67.5 112.5  # limits of omega intervals [deg]
crystal_system cubic
##### Number of refinement cycles
cycle 20
##### Outlier rejection information
min_refl 45        # NB! Use only grains with high completeness
rej_ia 0.2
rej_resmedian 5
rej_resmean 10
rej_vol 5
##### Global parameters
w 1                # Fit omega stage tilt parameter wy
tilt 1             # Fit detector tilt parameters tx, ty, tz
pixel 0            # Do not fit pixel size px and py
center 1           # Fit beam centre on detector along y-axis, cy
L 1                # Fit sample-to-detector distance
##### Grain parameters
xyz 1              # Fit grain positions
rod 1              # Fit orientations and thus Rodrigues vectors
eps 0              # Fit strain tensors
##### Tolerances
tol_global 1e-1
tol_rotpos 1e-2
```

5 Output

All output files will be saved in a directory with the name of the used input file up to the first punctuation, so in the example using `fitallb.inp` as input file, the output directory will be named `fitallb`. This directory name will also be used as the stem of the generated output files which are given in Table 5.

The parameters `eps11`, `eps22`,... are the components of the strain tensor in the Cartesian grain coordinate system; `eps11_s`, `eps22_s`,... are the strain tensor components in the sample system; `sig11`, `sig22`,... and the the components of the stress tensor in the Cartesian grain coordinate system; and finally `sig11_s`, `sig22_s`,... are the strain tensor components in the sample system.

The python wrapper for applied MINUIT variable metric minimisation, `pyminuit` (<http://code.google.com/p/pyminuit/>), puts certain limitations on how the function FCN to be minimised (1) is implemented. To make sure that the function has the right specifications it is necessary to build it before every refinement step. The building is performed by the `build_fcn.py` script, and the result is a file called `fcn.py` placed in the output directory (in our example `fitallb`) which contains the functions to be minimised in the correct syntax. `fcn.py` is read by the program during execution, but deleted upon normal termination of the fitting.

Besides generating the described output files (in directory `fitallb`), the program will give a lot of info in the dialog window from which it was called (standard output). To start out with the number of reflections rejected based on the different criteria are listed. Later on follows list of all grain with the number of assigned reflections, the total contribution to (1) from each grain and the average contribution per per reflection (should be roughly 3 according to the arguments in Section 2.3). While the program is running a counter specifies which grain is being refined now to give an idea of the refinement progress.

The quality of the fit can be judged from the `fitallb_log.log` and the standard output. Likewise the mean `IA` given in the `.gff` can be used as an indication in this direction.

Table 5: List of output files from fitallb.py, fitglobalgrain.py and fitglobal.py

file	contents
fitallb_log.log fitallb_near_log.log	Main output files for far- and nearfield: Global parameter values and standard deviations Residual values, refinement times and number of outliers for each refinement step
fitallb_rej.txt fitallb_near_rej.txt	List of rejected peaks and skipped grains for each refinement step. The reason to reject the peak, i.e. intensity or residual, is specified
fitallb_cor.txt fitallb_near_cor.txt	Correlation matrix of the refined parameters for each grain New matrices appended after each grain and final step
fitallb_cov.txt fitallb_near_cov.txt	As fitallb_cor.txt, except this is the covariance matrices
fitallb_global.txt	Correlation and covariance matrices of the refined global parameters are appended to this file after each cycle
fitallb_globals#_fab.par	ImageD11 type detector.par file with refined global parameters
fitallb.py: nearfield: fitallb_near_rotpos.gff farfield: fitallb_grain.gff fitallb_final.gff fitglobalgrain.py/ fitglobal.py: fitallb_rotpos#.gff	For each step in the algorithm the values of the parameters for each grain is listed in these (grain file format) files. Parameter order: grainno mean_IA grainvolume x y z rodx rody rodz U11 U12 U13 U21 U22 U23 U31 U32 U33 eps11 eps22 eps33 eps23 eps13 eps12 eps11_s eps22_s eps33_s eps23_s eps13_s eps12_s sig11 sig22 sig33 sig23 sig13 sig12 sig11_s sig22_s sig33_s sig23_s sig13_s sig12_s NB! If more than one final step is required the output file is overwritten in each step
fitallb_errors.txt	Estimated standard deviation of all the grain parameters given in the same order as listed above for the values. The file is updated after each refinement step. Step specific output files are names fitallb_step_errors.txt

6 Outlier rejection

Several different outlier rejection schemes are implemented into FitAllB, and the philosophy behind each of these will be outlined below. It should be noted that grains with less than a user defined number of assigned peak (min_refl) will be skipped to avoid spending time on refining non-physical ghost grains.

Median Absolute Deviation

Median absolute deviation (MAD) is used a robust measure for outlier rejection within FitAllB. Given the data set X_1, X_2, \dots, X_n the median absolute deviation is defined as:

$$\text{MAD} = \text{median}_i(|X_i - \text{median}_j X_j|)$$

For normally distributed data more than 99% of the observations should fall between the $\text{median} \pm 5\text{MAD}$. In FitAllB the method is used iteratively:

While more outliers are present in the data set

Calculate median and MAD of data set

Reject data point differing by more than $\text{madlimit} * \text{MAD}$ from median

6.1 Based on internal angles

The internal angle (measured in degrees) is the angle between $\mathbf{\Gamma}_{ij}^{-1} \mathbf{\overline{G}}_{ij}$ and $\frac{\lambda}{2\pi} \mathbf{U}_i \mathbf{B}_i \mathbf{\overline{G}}_{hkl,ij}$ of (1). All reflections with an internal angle greater than `rej_ia` will be rejected as outliers. The default value for undeformed materials is 0.2, this must be increased for deformed samples.

6.2 Based on intensities

This check is only carried out if a valid structure file is given in `fitallb.inp`. In this case the measure $\frac{I}{LP|F^2|}$ is calculated for each peak. Here I is the intensity, L is the Lorentz factor, P is the polarisation factor and $|F^2|$ is the theoretical structure factor squared determined based on the structure file. This quantity is directly proportional to the grain volume and should thus be roughly the same for all peaks assigned to a given grain. Thus a MAD outlier rejection with a `madlimit` of `rej_vol` is performed on these volume measures within each grain. The default value of 5 was chosen based on the arguments in MAD Section. Increasing the value will cause less reflections to be rejected. Reasonable values are found in [3;20].

6.3 Based on residuals

The residual is the refined quantity and should thus be as small as possible. Sometimes a single peak contributes abnormally much to the residual. This could either be because the peak belongs to a grain for which the parameters are still poor (in which case usually all peaks assigned to this grain will contribute rather much to the residual) or because the peak is assigned to a wrong grain. It is the peaks of this second kind that the residual based outlier rejection is tuned to spot and get rid of.

6.3.1 Based on residuals, robust

At any given time the contribution to the residual from each peak can be calculated. Within each grain the mean and median of these are determined and the peaks with the largest residual contributions are rejected until the mean is less than `rej_resmedian` times the median. The default value is 5, but any value in $]2;\infty[$ can be used, the larger the value the less reflections are rejected.

6.3.2 Based on average residuals

After each refinement step the peaks contributing more than `rej_resmean` (default=10) times the mean peak contribution to the residual within each grain are rejected. This specific outlier rejection scheme is, contrary to the others, not used until after the first refinement step as it is not very robust towards poor starting values of the grain parameters. Values in $[5;20]$ are applicable in most cases.

6.4 Peaks assigned to multiple grains

Occasionally a number of peaks will be assigned to more than one grain, especially if many grains are illuminated simultaneously, the sample is textured or very loose cuts have been applied in the GrainSpotter indexing or the FitAllB forward projection (Section 3.2.1). FitAllB identifies these peaks and looks at how they contribute to each of the assigned grains. If it is found that the peak gives rise to a higher residual in grain1 than in grain2, and at the same time the volume calculated for the peak is further from the mean volume in grain1 than in grain2, then the peak will be rejected from grain1. This feature can be turned off (default: on) by setting `rej_multi` to 0. This is for instance done for refinements of twinning samples where the different twin variants share a number of reflections.

6.5 Merging of grains

It sometimes happens that the GrainSpotter comes up with two grains that are said to be different but in fact have the same orientation and many of the same peaks assigned. FitAllB contains a routine for identifying and merging grains of this type. In `fitallb.inp` the `overlap` command tells how large a fraction of overlapping peaks is allowed before the grains are considered to be identical. The default value is 1, i.e. do not merge anything. Grains where a larger fraction of the assigned peaks are identical are cornered out and the grain with the fewest assigned peaks is skipped. In case the two grains contain the same number of peaks, only the identical peaks are kept in the refinement.

7 Installation and execution

The newest development version of FitAllB can be obtained from the subversion (SVN) repository:

```
svn co https://fable.svn.sourceforge.net/svnroot/fable/FitAllB
```

Go to the trunk and install the program by:

```
python setup.py install
```

NB! Most likely this has to be done with root privileges, e.g. put a `sudo` in front of the command.

Alternatively a packed version called `FitAllB-1.0.0.zip` can be downloaded from

```
https://sourceforge.net/project/showfiles.php?group_id=82044
```

Go to `FitAllB-1.0.0` and install the program by:

```
python setup.py install
```

NB! Most likely this has to be done with root privileges, e.g. put a `sudo` in front of the command.

7.1 Required packages

python 2.4 or later (<http://www.python.org>)

pyminuit (<http://code.google.com/p/pyminuit/>)

PIL (<http://www.pythonware.com>)

numpy (<http://www.numpy.org/>)

scipy (<http://www.scipy.org/Download>)

PyCifRW (anbf2.kek.jp/CIF/)

From FABLE: ImageD11, xfab, PolyXSim, fabIO

7.2 Execution

After setting the relevant paths the program can then be called from the directory containing the main input files (here .inp) in the following way:

```
fitallb.py -i fitallb.inp
fitglobalgrain.py -i fitglobalgrain5_5.inp
fitglobal.py -i fitglobal5_5.inp
```

7.3 Provided test examples

All files required to perform the below describe test runs are found in trunk/test.

if10.inp: (fitallb.py, near- and far-field data)

10 grains of IF steel simulated using PolyXSim within an illuminated volume of $0.7 \times 0.7 \times 0.01$ mm with random orientations, grain sizes and Gaussian strains with a mean of 0 and a spread of 0.001. The refinement is an example of using both near- and far-field data, and the runtime is approx. 1 min per grain on a 2.2 GHzm 3.5 GB RAM PC.

if10_res.inp: (fitallb.py, far-field data only, resumed refinement)

Same data as for if10.inp, but only the far-field refinement is performed. The starting values of all grain parameters is read from the if10_near_rotpos.gff file generated in the if10 refinement to show how resuming a refinement can be done. Note that the grain positions refined on the near-field detector are kept fixed in this far-field refinement. Runtime approx. 40 sec per grain.

fitglobalgrain5_5.inp: (fitglobalgrain.py)

5 grains of undeformed IF steel simulated within a volume of $0.7 \times 0.7 \times 0.01$ mm with random orientations and grain sizes. The input file of global parameters, if100_globals_wedge.par, has a slight offset in all of these as compared to the values used to simulate the diffraction images to demonstrate the powers of the fitglobal-grain.py. The true parameters used for the simulation are given in if100_globals_wedge_true.par for comparison. 5 refinement cycles performed. Runtime: 14 min.

fitglobal5_5.inp: (fitglobal.py)

Same input as for fitglobalgrain5_5, but intended for use with fitglobal.py to demonstrate the different between the two. Runtime: 16 min.

fitglobal5_res2.inp: (fitglobal.py)

Resuming the fitglobal refinement of fitglobal5_5 using as input the final grain parameters, fitglobal5_5_rotpos4.gff, and globals, fitglobal5_5_globals4_fab.par, as input to do 2 more cycles. Runtime: 5 min.

7.4 Contact

For more information on the standard 3DXRD geometry the user is referred to the geometry document [Poulsen et al., 2009]. Furthermore FitAllB has its own wiki with input examples and links to useful stuff: (<http://fable.wiki.sourceforge.net/FitAllB>).

Questions, comments and suggestions are most welcome!

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