

2025 FullProf School

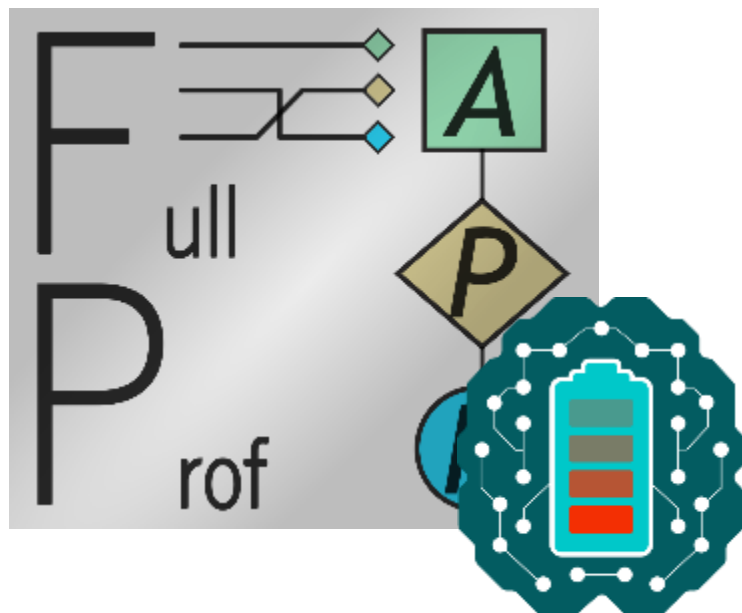
Introduction to FullProfAPP

Monday, March 31st 2025

Oier Arcelus

> APP DESCRIPTION

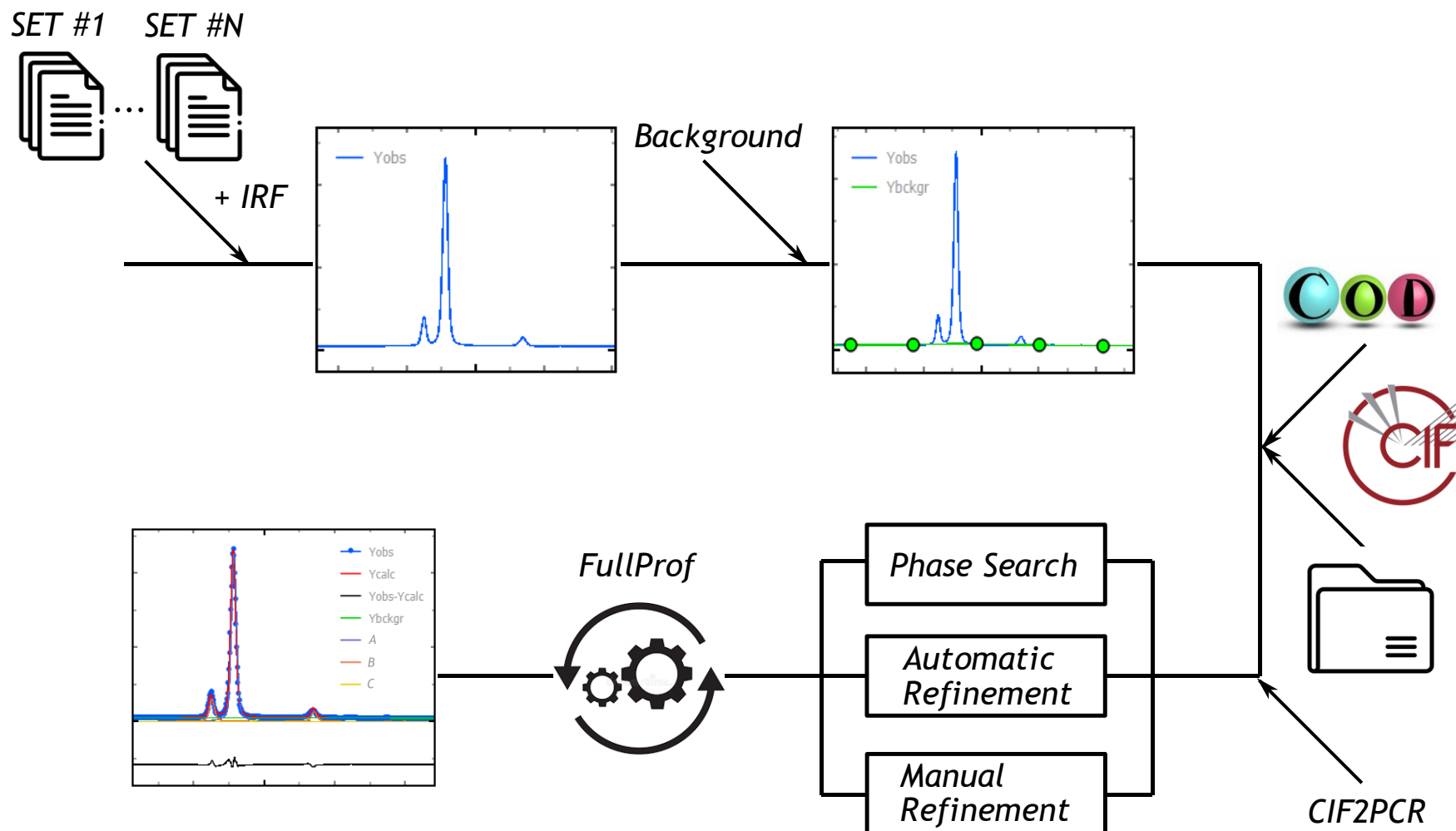
COLLABORATORS



> APP DESCRIPTION

WHAT IS IT?

- A **Graphical User Interface (GUI)** for **FullProf** built in Python.
- Provides **automated** protocols to treat large **batches of data**.



> APP DESCRIPTION

WHAT IS IT NOT?

- It is **NOT** a **superset** of FullProf.
- Full compatibility is not achieved yet. You **cannot do**:
 - Symmetry mode analysis
 - Magnetic structures
 - Single crystal diffraction
 - Simulated annealing
 - ...
- Take **special care** when loading **external** PCR files, behavior might be unexpected.
- You **CAN** however perform a bit more advanced analysis:
 - Anisotropic size broadening
 - Anisotropic strain broadening
 - Anisotropic thermal parameters for crystallographic sites
 - Bond-Valence Sum (BVS) calculations
 - ...

> INSTALLATION

STEPS

- Have the last version of **FullProf Suite** installed
 - <https://www.ill.eu/sites/fullprof/php/downloads.html>
- Download **FullProfAPP!**
 - <https://www.ill.eu/sites/fullprof/php/downloads.html>
 - For **Windows:**
 - Run the installer executable
 - For **Linux:**
 - Run the command **dpkg -i fpapp_linux_installer.deb**
- **Manual:**
 - <https://fullprofapp.readthedocs.io/>
- **Contact:**
 - **fullprofapp@cicenergigune.com**

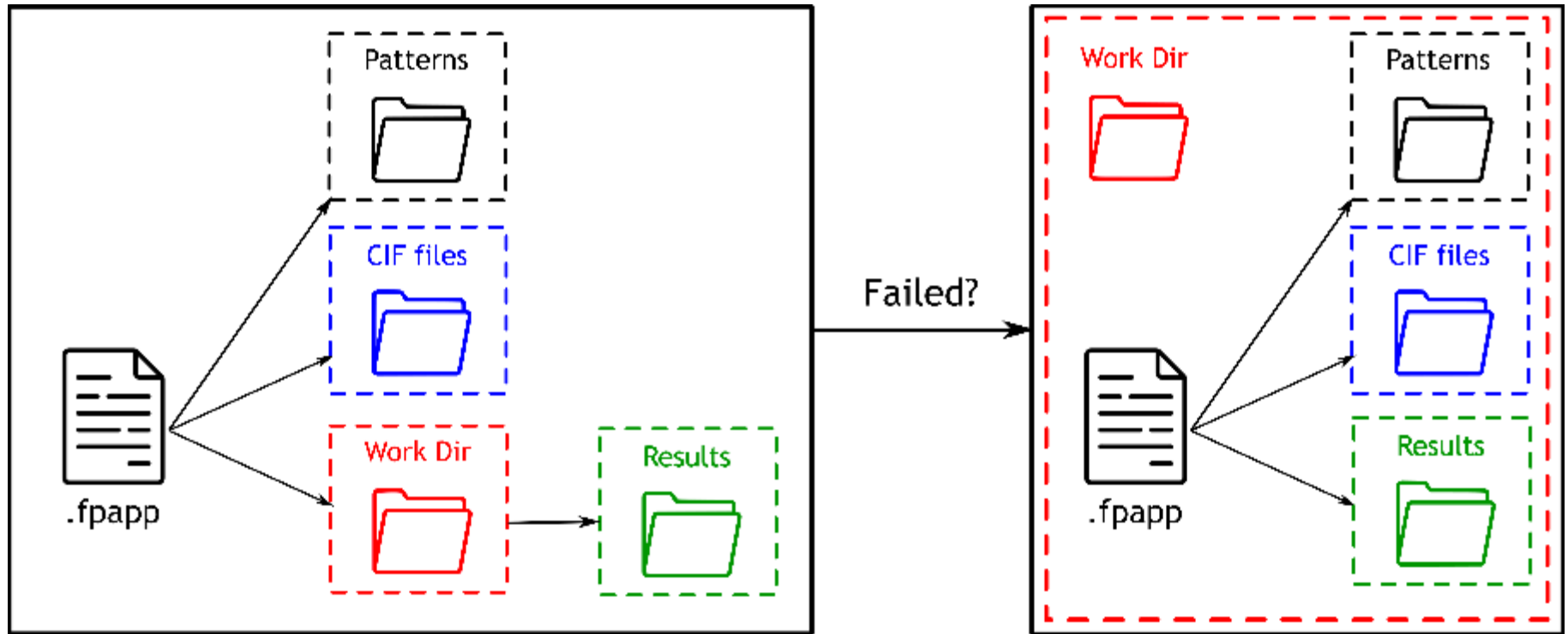
> WALKTHROUGH

GRAPHICAL USER INTERFACE

EXECUTE THE PROGRAM!

> WALKTHROUGH

GRAPHICAL USER INTERFACE



> WALKTHROUGH

GRAPHICAL USER INTERFACE

COLUMNS: MULTIPATTERN REFINEMENT

ROWS:
PATTERNS
SEQUENCE

PATT #1	PATT #2	...	PATT #N
File1-1	File1-2	...	File1-N
File2-1	File2-2	...	File2-N
...	...	...	...
...	...	...	...
...	...	...	...
FileN-1	FileN-2	...	FileN-N

> WALKTHROUGH

GRAPHICAL USER INTERFACE

	PATT: 0	PATT: 1
1	XRD_f00002.xye ☐	NPD_f00002.xye ☐
2	XRD_f00003.xye ☒	NPD_f00003.xye ☒
3	XRD_f00004.xye ☐	NPD_f00004.xye ☒
4	XRD_f00005.xye ☒	NPD_f00005.xye ☐

> WALKTHROUGH

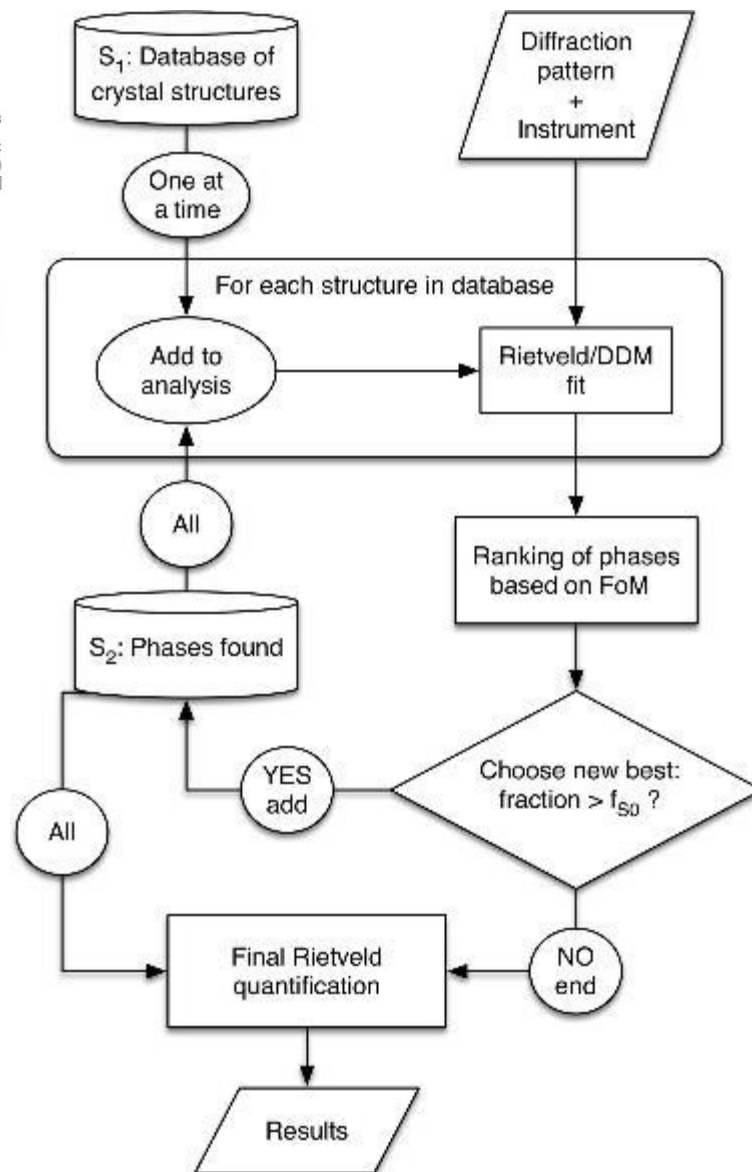
GRAPHICAL USER INTERFACE

Full-profile search-match by the Rietveld method

Luca Lutterotti,^{a,c*} Henry Pilière,^b Christophe Fontugne,^b Philippe Boullay^c and Daniel Chateigner^c

^aDipartimento Ingegneria Industriale, Università di Trento, Italy, ^bThermo Fisher Scientific, INEL SAS, Artenay, France, and ^cCRISMAT - ENSICAEN, Université de Caen Normandie, Normandie Université, France

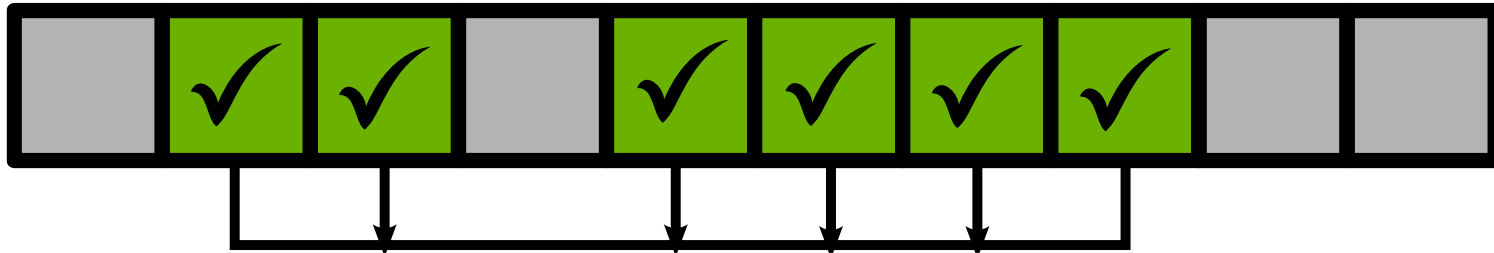
$$FoM^p = \left[\frac{1}{R_{wp} + a v_0^p \left| \frac{1}{v_r^p} - \frac{1}{v_0^p} \right|} + b (100 - f_r^p) \right] \left(1 + \frac{c}{\langle D^p \rangle} + d \varepsilon^p \right)^{-1}$$



> WALKTHROUGH

GRAPHICAL USER INTERFACE

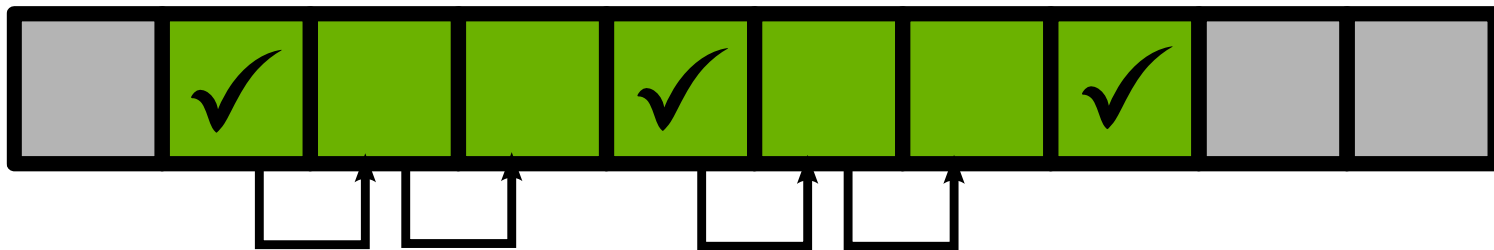
Normal Mode



Each job is run independently

- Need to load materials for each one
- Parallelized operation of checked jobs

Sequential Mode



Jobs are run sequentially

- Sequence is split over checks (checkpoints)
- Each chunk runs in parallel
- Each chunk mixes phases that appear on the checkpoints

GRACIAS · THANK YOU · ESKERRIK ASKO

CIC **energig**UNE

MEMBER OF BASQUE RESEARCH
& TECHNOLOGY ALLIANCE

Parque Tecnológico · c/Albert Einstein 48
01510 Vitoria-Gasteiz · (Álava) SPAIN
+34 945 29 71 08

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