2023 FullProf School

Introduction to FullProfAPP

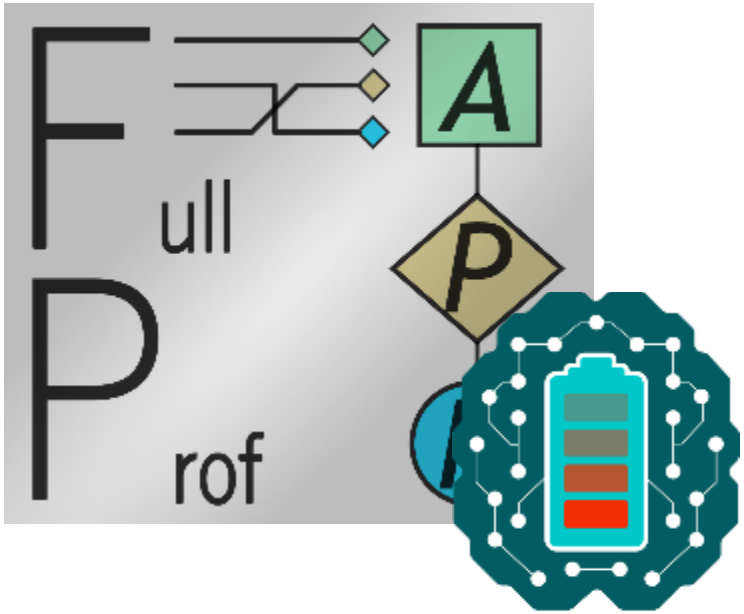
Monday, October 2nd 2023

Oier Arcelus

CIC energiGUNE
MEMBER OF BASQUE RESEARCH & TECHNOLOGY ALLIANCE

> APP DESCRIPTION

COLLABORATORS





ICMAB
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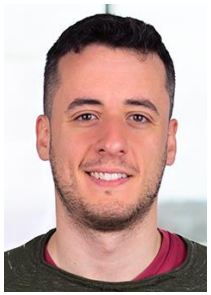
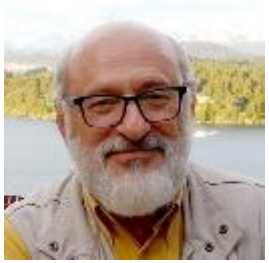
G-MAP

NEUTRONS FOR SCIENCE®

ALBA

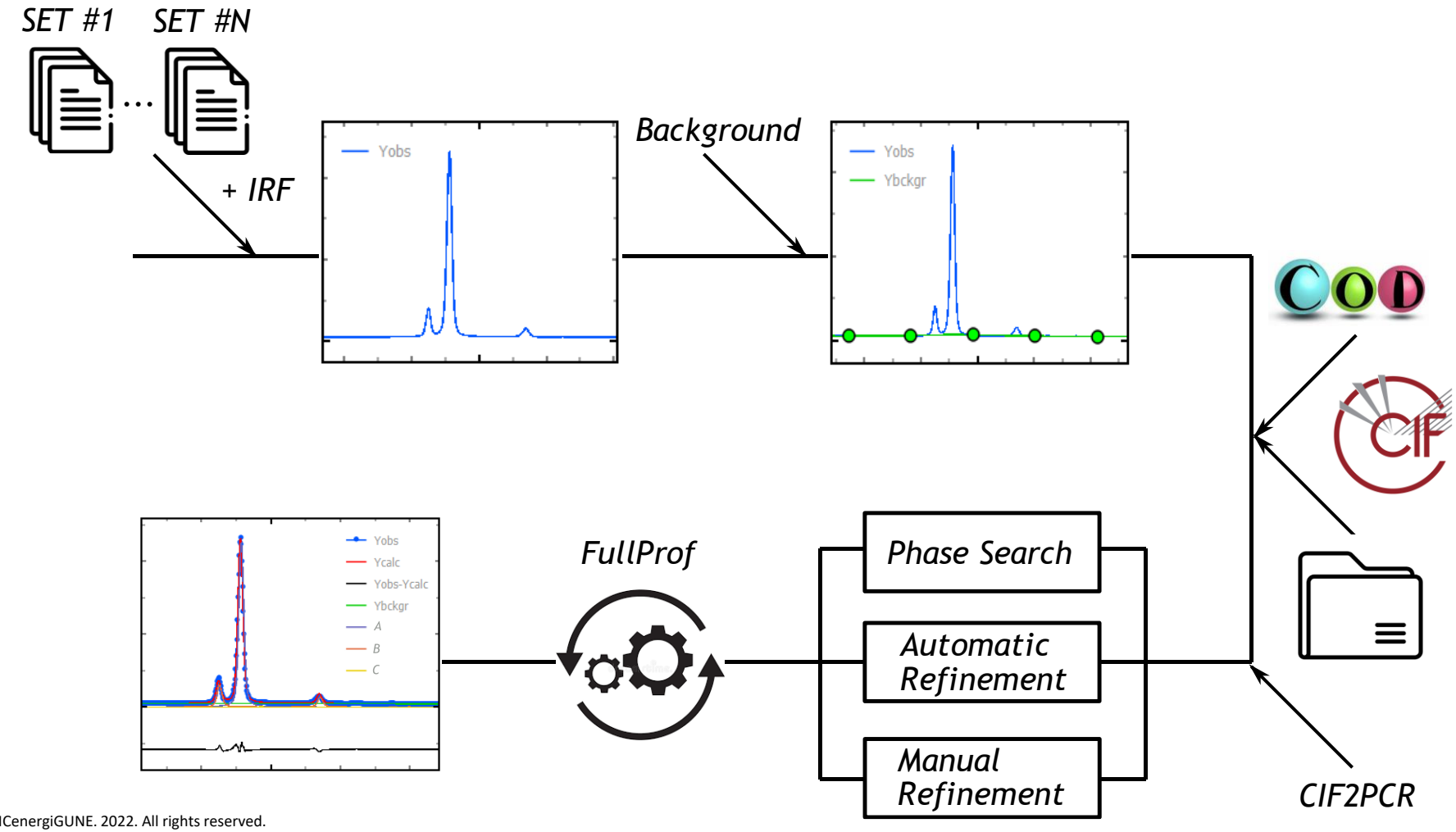



APP DESCRIPTION

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**

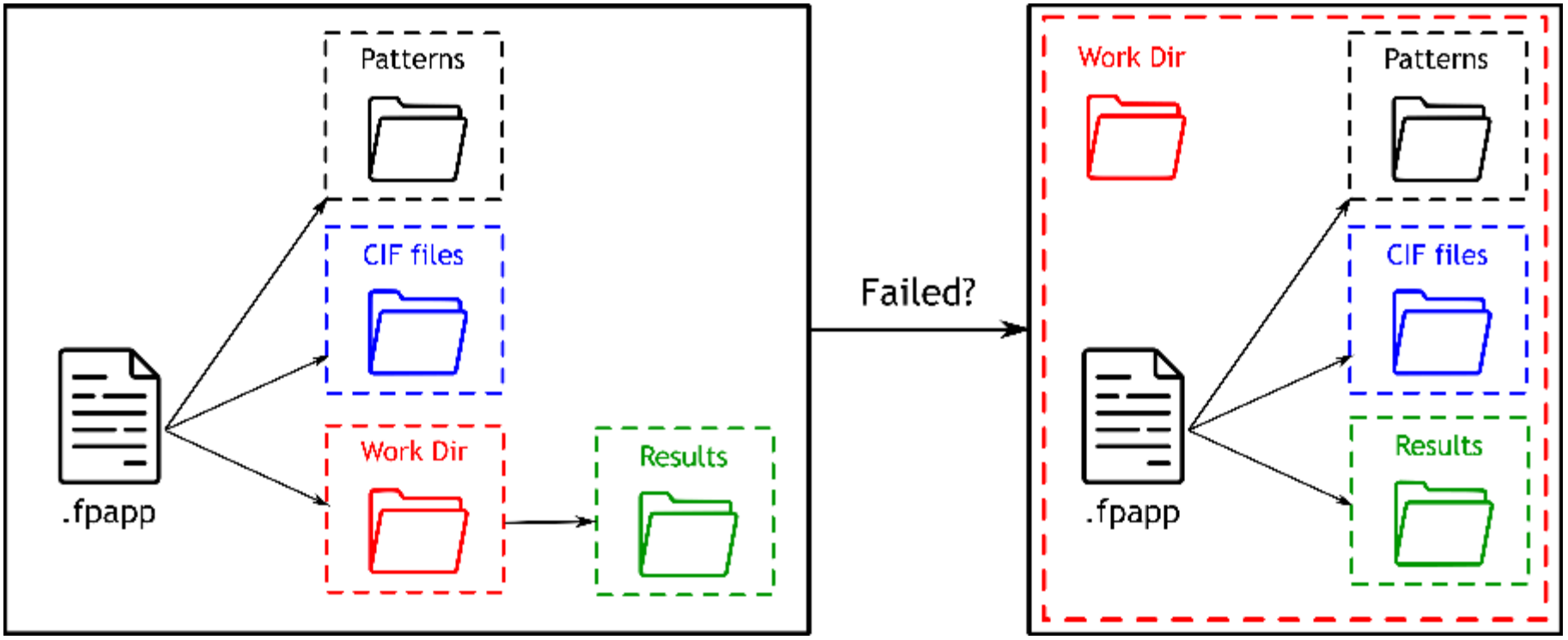
WALKTHROUGH

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

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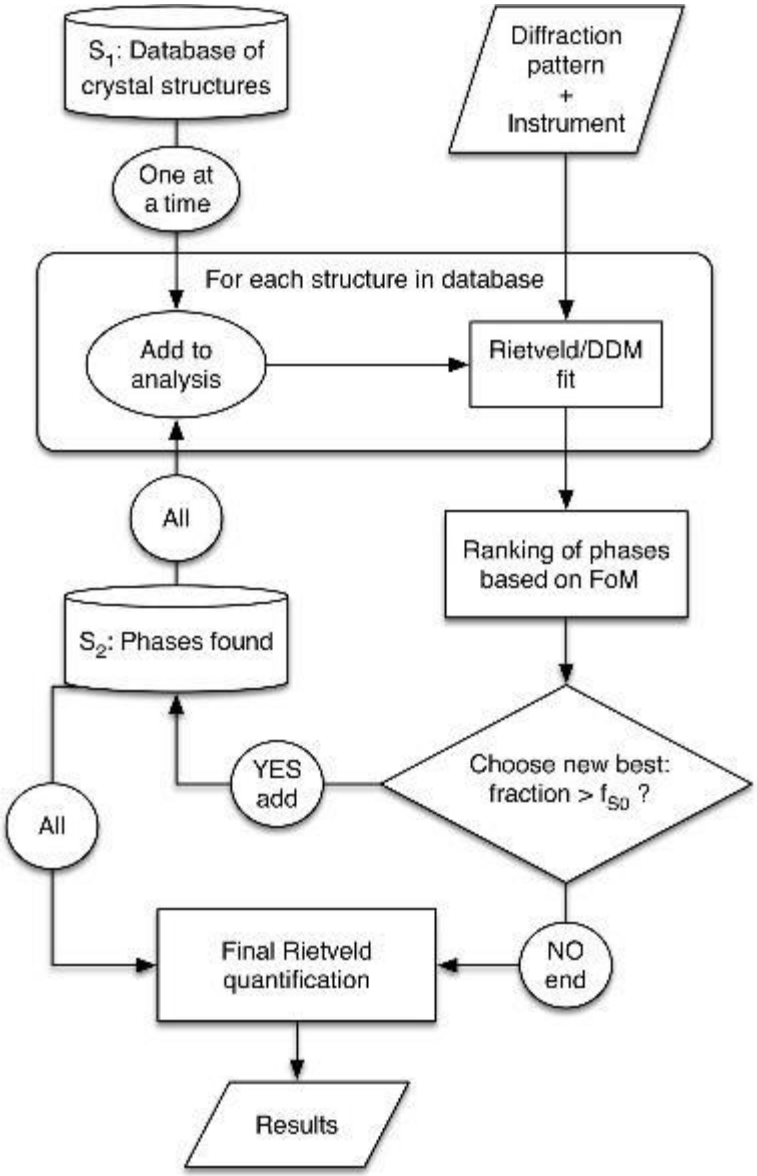
Full-profile search–match by the Rietveld method

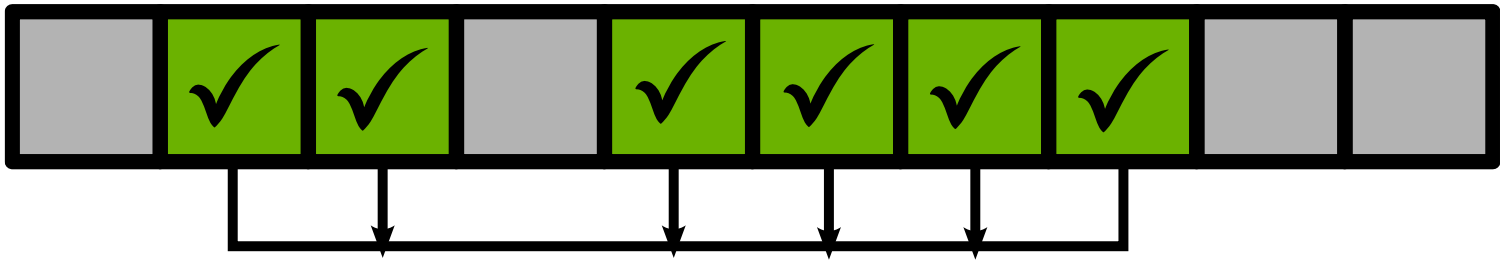
Luca Lutterotti,[a,c]* Henry Pillière,[b] Christophe Fontugne,[b] Philippe Boullay[c] and Daniel Chateigner[c]

[a]Dipartimento Ingegneria Industriale, Università di Trento, Italy, [b]Thermo Fisher Scientific, INEL SAS, Artenay, France, and [c]CRISMAT – ENSICAEN, Université de Caen Normandie, Normandie Université, France

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

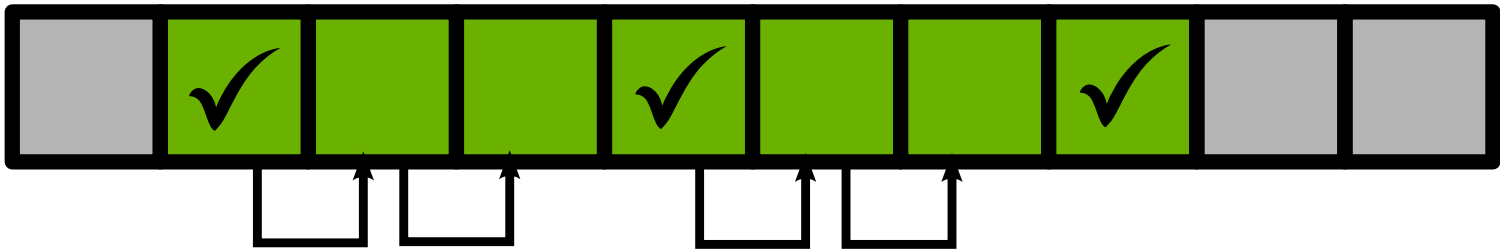


Normal Mode



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

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