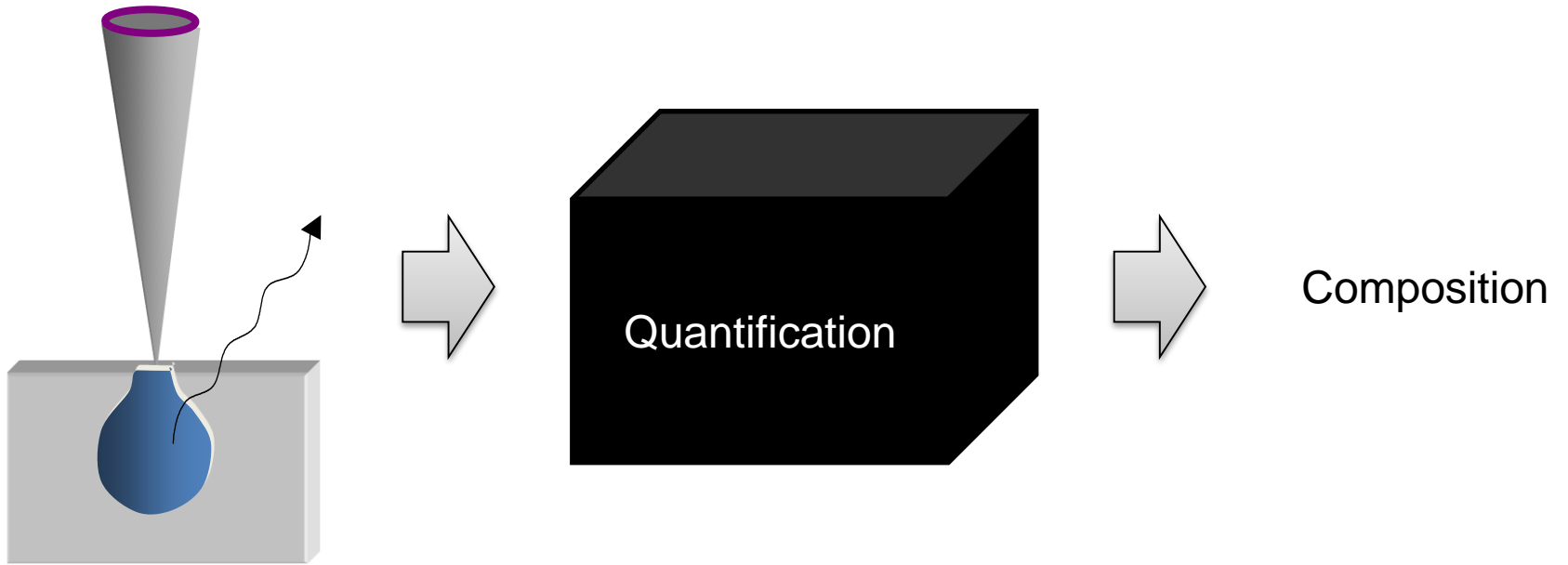


Discussion forum on open source software for quantitative microanalysis

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Presentation of project



Presentation of project

- community-driven
- open source
- centralize physical quantity databases and algorithms used for quantification
- encourage collaborative work
- provide the necessary building blocks for new projects in microanalysis

Justifications

- If someone now wants to develop a new quantification routine, one must write code to
 - Handle different x-ray transitions
 - Mass absorption coefficients
 - Ionization potential
 - Surface ionization
 - Backscatter factor
 - Stopping power
 - Etc.
 - Iteration algorithm
 - Read / handle experimental data



Justifications

Scientific publishing

- Transparency
 - Published
 - Accessible by any research
- Quality
 - Peer reviewed
- Validation
 - Peer reviewed
 - Verifiable results

Open source project

- Transparency
 - Code is always accessible
 - Any modification is stored
- Quality
 - Report bugs
 - Controlled by maintainers
- Validation
 - Test for consistency
 - Test against known experimental values
 - Bug reporting mechanism

Software

Software	Year	Author	License	Model(s)
GMRFilm	1993	Waldo	Open source	PROZA, PAP
CITZAF GUI	1995	Armstrong/Davis	Free	CITZAF
MULTI	1999	Trincavelli	Free	PAP,PROZA,
Esprit	2015	Bruker	Commercial	ZAF, XPP
PeakSight	2015	Cameca	Commercial	XPHI?
TEAM	2015	EDAX	Commercial	ZAF?
PC-EPMA	2015	JEOL	Commercial	ZAF, PRZ?
Aztec	2015	Oxford	Commercial	XPP?
CalcZAF	2015	Probe Software	Free	ZAF, PAP, XPP, PROZA, CITZAF
Probe for EPMA	2015	Probe Software	Commercial / source available	ZAF, PAP, XPP, PROZA, CITZAF
Xone	2015	Quartz	Commercial	ZAF?, PRZ?
DTSA-II	2015	Ritchie / NIST	Open source	ZAF, PAP, XPP, PROZA, CITZAF
IDFix	2015	SAMx	Commercial	?
STRATAGem	2015	SAMx	Commercial	PAP, XPP
Noran	2015	Thermo Scientific	Commercial	PROZA
Hyperspy	2015	de la Peña et al.	Open source	Cliff-Lorimer

+ all non-distributed personal / research group codes

Requirements for open source projects

- Website
- Mailing list
- Version control
- Code proposal / personal fork
- Bug tracker
- Wiki / Documentation
- Continuous integration (testing)
 - Validation with experimental data
- Release system

Source: Fogel (2010) Producing Open Source Software

Project organization

- **Members**
 - **Maintainers:** Organizing the project, managing bug reports
 - **Programmers:** Writing code
 - **Contributors:** Donate their own code to the project
 - **Experts:** Review algorithms used, contribute equations and databases
 - **Users:** Any scientist that may use or use a derivative product from this library
- **Communication strategies**
 - Approval cycle for changes
 - Decision of priorities
 - Distribution of workload

Milestones

- Selection of programming language(s)
- Selection of license
- Setup of the source code hosting platform
- List of parameters required to implement
 - Fundamental parameters
 - Matrix correction algorithms
 - Quantification procedures
 - Spectrum analysis routines
- Possible sources of funding