

Eval15 integration

Martin Lutz
Crystal and Structural Chemistry
Bijvoet Center for Biomolecular Research
Utrecht University
The Netherlands

m.lutz@uu.nl

<http://www.cryst.chem.uu.nl/lutz>

A.M.M. Schreurs, X. Xian, L.M.J. Kroon-Batenburg,
J. Appl. Cryst. (2010). **43**, 70-82.

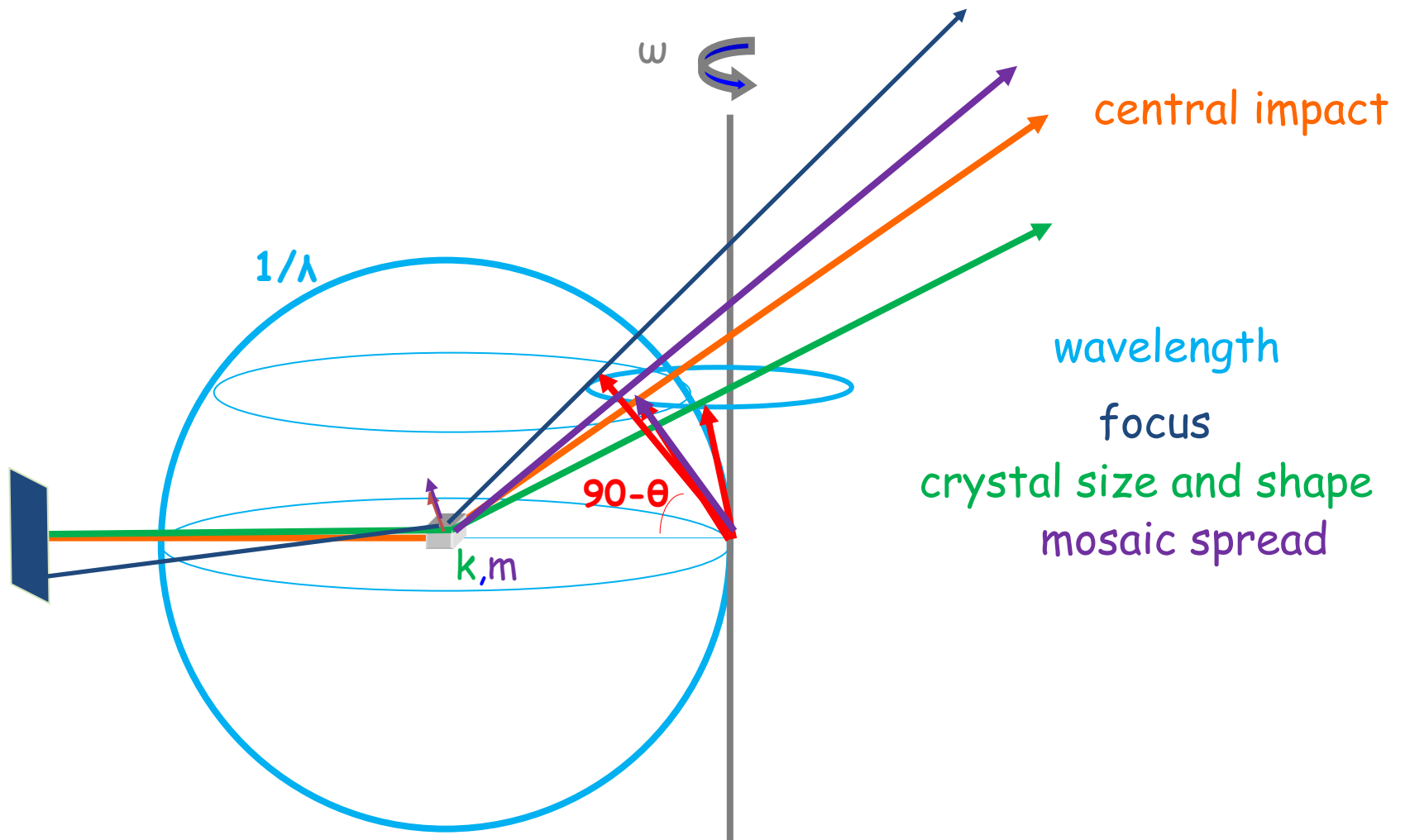
Introduction

- Academic development
- Aim: meet the requirements of the researcher
- Aim: data quality
- Aim: deal with “standard” cases
- Aim: deal with “difficult” cases
- Lower priority: user interface
- Lower priority: speed

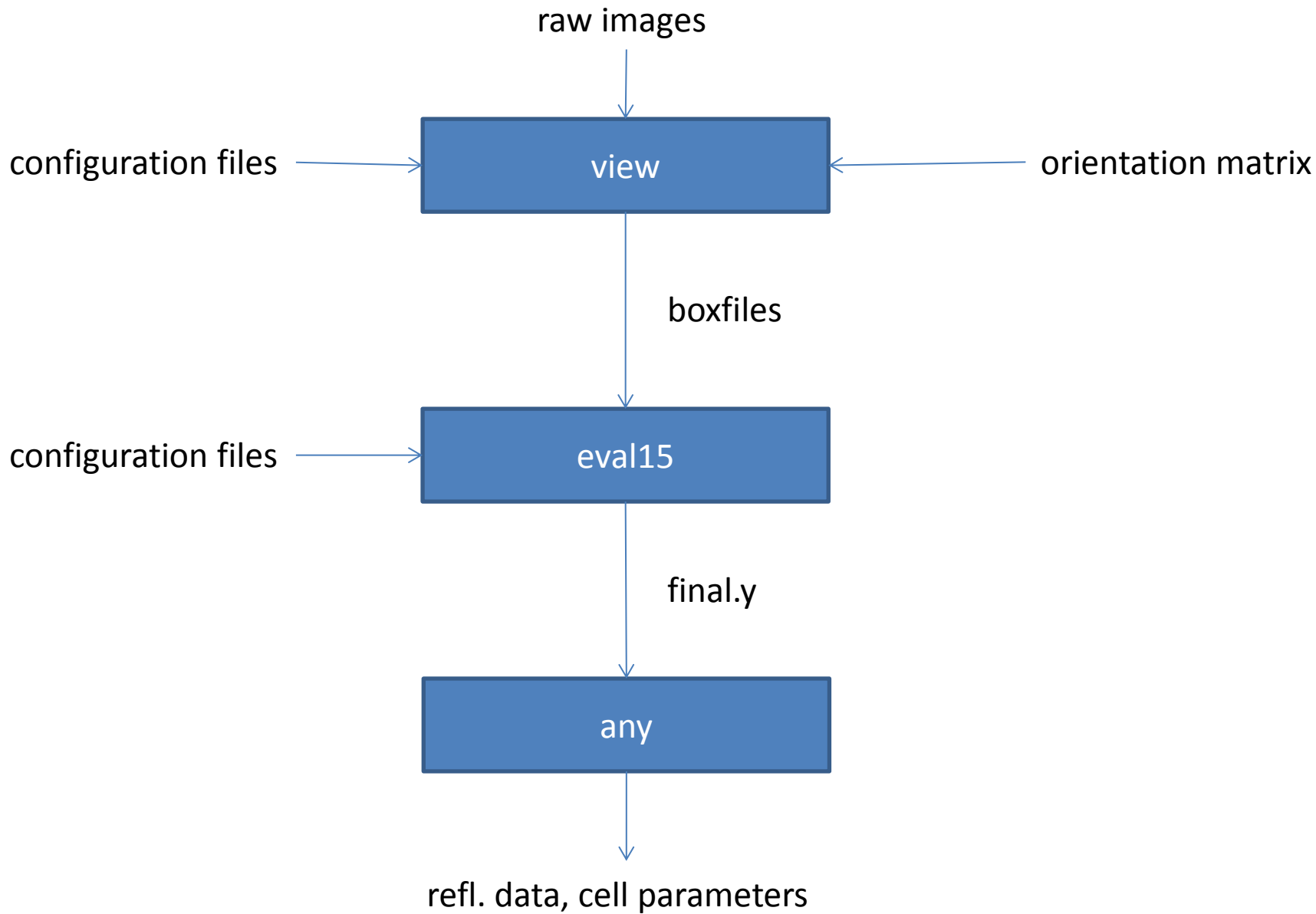
General impact

ω rotation to Bragg condition at ζ :

$$\cos \zeta = (\sin \theta - \sin \chi_{\text{f}k}) / (\cos \chi_{\text{f}k} \cos \chi)$$



Program flow



view

- View raw images
- Peak search
- Create boxfiles
- Helper applications

configuration files for “view”

- `detalign.vic`
- `goniostat.vic`
- `beamstop.vic`
- `[view.init]`

Peak search with “view”

- Create macro files for “view” using `buildsearch`
- `view @isearch`
- Result files:
 - name.drx
 - name.pk

dirax

- Indexing program
- A.J.M. Duisenberg (1992). *J. Appl. Cryst.* 25, 92-96
- Input file:
 - name.drx
- Result file:
 - name.rmat

peakref

- Refinement of orientation matrix and diffractometer configuration
- Input files:
 - name.rmat
 - name.pk
- Result files:
 - name.rmat
 - detalign.vic, goniostat.vic

rmatrix

- Find standard setting of unit cell (Bravais centering)
- Input file:
 - name.rmat
- Output file:
 - name.rmat

Create boxfiles with “view”

- Create macro files for “view” using `builddatcol`
- `view @datcol`
- Result files:
 - `*.shoe`

Integrate the boxfiles

- Create Eval15 configuration files with `buildeval15`
- Interactively check the profile prediction with `eval15`
- Integrate all boxfiles with `eval15all`

“Parallel processing”

- You can use different processors for the integration
- Create a file `~/hosts` which contains the computernames for login with ssh (with passkey)
- Alternatively create a file “computers” in the local directory
- `batchsetup set`
- `batchstart`

Queing system

- If you are using Eval15 regularly on a computer cluster, we recommend to use the **gridengine** (probably included in your linux distribution)

any

- any read final.y.gz
- hklf4 (writes reflections in SHELX format)
- pk (writes impact positions for peakref)

Helper programs related to “view”

- tunebeamstop
- scancheck / scancheckplot
- buildsc / scanplot
- imagesum
- low3
- buildrest
- buildphichi

Helper programs related to unit cell

- rmatrix
- cell
- cellplot
- 2view
- p4p2rmat

Helper programs for reflection data

- anafcf
- loglog
- mergehklf5
- plotcosines