REFSANS@MLZ instrument
(meta-information for reference catalogs)

ORSO Meeting
2023-06-21

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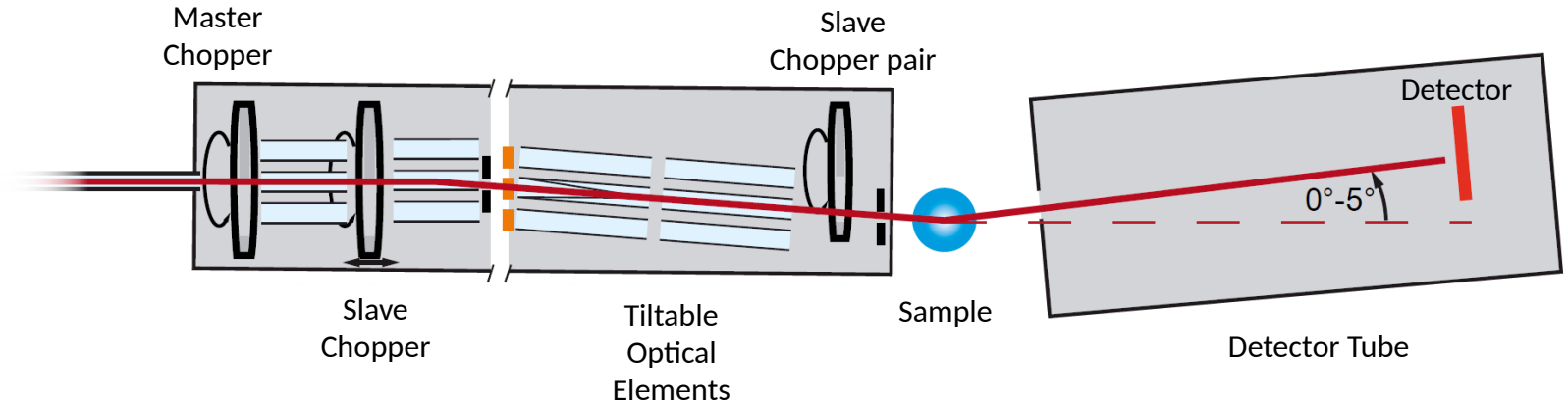
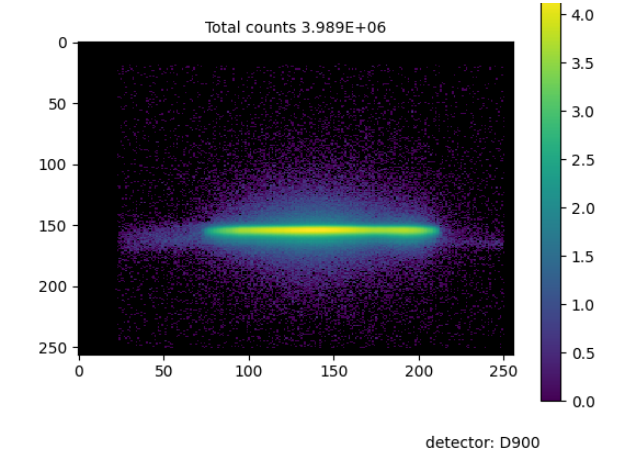
The REFSANS Instrument: Neutron Reflectrometry (& GISANS)

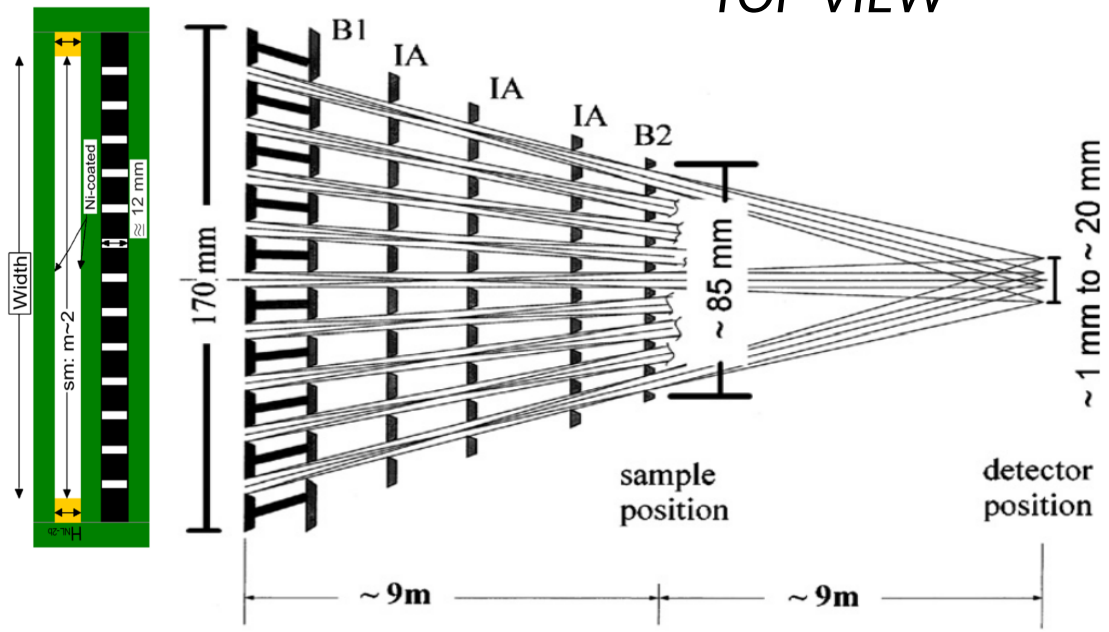


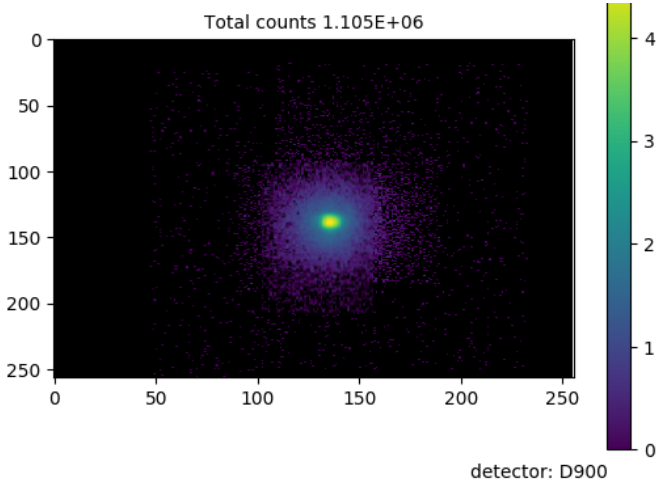


- TOF & List-mode acq: retrospective/adaptable binning of wavelength and time (kinetics)
- λ-resolution and -range: tunable from 1-10% and (usually) from 3 – 21 Å
- typical Q_z range: 0.005 – 0.25 $Å^{-1}$
- beam divergence: Independent control of horiz. / vert. divergence
- liquid interfaces: beam tiltable by up to 2.75°
- beam cross section: max. 80 x 12mm on sample

The REFSANS Instrument: (GISANS Option:)

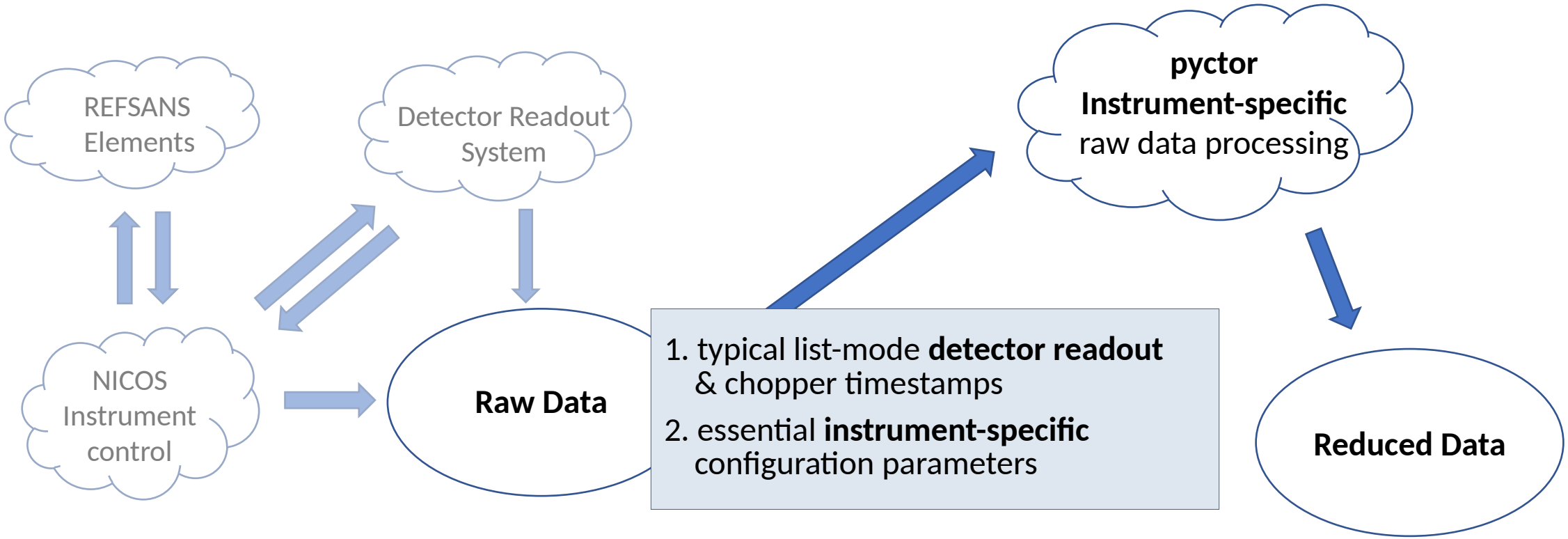
TOP VIEW





- Radially collimated beam focused on the detector active area, at ~ 9m from the sample.
- Possibility to move the detector laterally, for an asymmetric Q_y range
- typical Q ranges: Q_z 0.005 – 0.25 $Å^{-1}$; Q_y 9.5×10^{-5} – 0.18 $Å^{-1}$

The REFSANS reduction workflow:



most of the (essential) raw meta&data is only useable in the context of deep knowledge of the specific (often unique) instrument design

The REFSANS meta-data groups:

- [global] : general user/experiment/sample information
- [shutter] : list, open/closed
- [chopper_config], [chopper]: chopper speed, positions, mode, disc phases & positions, ..
- [optic], [NOK_mode], [NOK_position], [slit_mode], [slit_position]: optics & beampath configuration details
- [polarizator] : status, flipper, direction
- [sample] : collimator, goniometer, slits, samplechange, sample dimensions
- [detector] : geometry/alignment
- [vacuum] : pressures
- [se_...] : sample environment system(s) parameters
- [monitor]
- [Extra]

The relevant meta-data categories, qualitatively:

- **classic user/facility/proposal metadata**
- **classic reflectometry meta-data**
  - q ranges / angles / wavelengths,
  - sample tilting vs setup tilting,
  - beam collimation & footprint on sample
- **instrument information:**
  - probe (neutrons/x-rays): relevant to contrast, flux, resolution and specific reduction steps
  - 2D / 1D detector, dector type (w.r.t specific corrections required)
  - Q selection technique: monochromator vs TOF (neutrons)
  - (neutrons.) horizontal vs. Vertical geometry, affects ballistic corrections (and resolution)
- **reduction information:**
  - employed peak fitting models/methods
  - ballistic correction models (e.g. explicit modeling vs. cancellation-of-effects)
  - beam fluctuation compensation (monitor, none, error estimation)

Relevant Reference-Data Information:

- **General** (derived) **method specific information** such as e.g. wavelength & resolution
- **Sample:** information / **persistent** reference to sample/**documentation**
- **Instrument identifier** + **DOI** of applicable **description**
  of the **present (unique) instrument design**/parameters and its related data evaluation concept
- **Raw data** with applicable **instrument specific parameters**
  (such as e.g. chopper and slit configurations, or monochromator, etc; and beam monitor / error information)
- **Analysis script** transforming instrument-specific raw data
  to method specific "universal" format (e.g. Reflectivity/Signal vs. Q)
- If not part of the script, **persistent reference** to
  a (versioned/reproducible, e.g. git) repository of the **required libraries**
- If applicable / not covered by the instrument description,
  a **DOI** to the description of the instrument/software specific raw **data reduction steps** (here: pyctor)
- If applicable: **documentation** of custom / manual **parameter choices**
  e.g. custom fit models, or specific ballistic trajectory correction method