

Generic Reduction Procedure

- 1) READ INPUT:
User input: Runnumbers (REF, DB, WATER, INST BACK)
Metadata: slits, detector angle, sample angle, MONITOR, TIME ...
User input data: foreground range, background range, wavelength range, grouping,
Detector: 2D, line, 1D
- 2) Determine Measurement Type
A: TOF (POL or UPOL)
B: MONO (POL or UPOL)
- 3) Determine if kinetic / streaming
- 4) Determine XYZ coordinate of axis
IF detector XY: Integrate loose collimation direction
IF MONO: determine scan axis, stack data on scan axis direction
- 5) Sort or group measurements to measurement type
NOTE: different measurements can be stored in 5th dimension:
1: x-axis, 2: y-axis, 3: intensity, 4: polarization, 5: time/streaming/temperature/fields/etc...
IF MONO: sort scan axis, sort polarizations, sort measurements in sequence
IF TOF: sort polarizations, sort angles, sort measurements in sequence
IF kinetic: loop through slices
IF streaming: sort cyclic data and average similar input
- 6) Calculate errors and propagate appropriately through following steps
- 7) Determine foreground (ROI) and background (back)
IF no DB: DB=monitor OR DB=1
NOTE: Here a binning can take place, but that requires calculating lambda, theta and the resolutions before.
- 8) Normalization:
slits, water, monitor/time
- 9) Subtract instrument background from REF and DB, subtract background from REF and DB (averaged or fitted)
- 10) Average data at similar XY coordinate
IF MONO: average same theta/2theta values
IF TOF: probably no further averaging
- 11) CASE: Gravity correction for horizontal reflectometer
- 12) Calculate missing axis theta, 2theta, lambda,
CASE: Reflection UP or DOWN in horizontal reflectometer
CASE: Coherent or incoherent analysis
- 13) Calculate angular width on detector of REF and DB => sample waviness for coherent
- 14) IF DB supplied: Integrate DB foreground
IF TOF: => 1D DB(lambda)
IF MONO: => 1D DB(scan axis)
- 15) IF POL: Correct 1D DB for polarization efficiency

- 16) Calculate 1D reflectivity:
 - CASE: incoherent
 - Integrate at constant λ over 2θ \Rightarrow 1D REF
 - Divide 1D REF by 1D DB \Rightarrow 1D REF/DB + E
 - CASE: coherent
 - Divide 2D REF by 1D DB column wise
 - Regroup data within new wavelength limits onto a given 2θ line
 - CASE: bent sample
 - CASE: divergent beam
 - \Rightarrow 1D REF/DB + E
- 17) IF TOF POL: loop to get all the polarizations to correct for efficiencies the 1D REF/DB as a function of λ
 - IF POL MONO: loop to get all polarizations to correct for polarization efficiency at fixed λ
- 18) Calculate resolutions in θ , λ
 - CASE: incoherent
 - CASE: coherent
- 19) Calculate Q
- 20) Group to a fraction of the Q resolution
 - NOTE: for the incoherent method it is possible here to use 1D REF(rebinned)/1D DB (rebinned)
- 21) Calculate 2D reflectivity in requested coordinates: QX/QZ, π/ϕ / $\theta/2\theta$
 - Divide 2D REF by 1D DB column wise
- 22) Perform polarization efficiency correction on all spin channels column wise
- 23) Update storage with direct beam
- 24) IF kinetic: loop over slices
- 25) IF multiple datasets: loop over 5th dimension
- 26) Perform final normalization corrections
- 27) Join data corresponding to 1 measurement
- 28) Store 1D and 2D outputs in readable format with metadata

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PHIa1    = 0.0114
PHIk1    = -0.0005
PHIk2    = 0.0014
PHIk3    = 0.0087
PHIk4    = 0.0121
PHIk5    = 0.0196
PHIxi1   = 8.1299
PHIxi2   = 13.0000
PHIxi3   = 16.1075
PHIxi4   = 20.0963
PHIyi1   = PHIa1+PHIk1*PHIxi1
PHIyi2   = PHIyi1+PHIk2*(PHIxi2-PHIxi1)
PHIyi3   = PHIyi2+PHIk3*(PHIxi3-PHIxi2)
PHIyi4   = PHIyi3+PHIk4*(PHIxi4-PHIxi3)

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xin=xinA[j]
;The efficiency at the lambda point:
;;**F1
if xin le F1xi1 then F1L[j] = F1a1+ F1k1*xin else $
if xin le F1xi2 then F1L[j] = F1yi1+ F1k2*(xin-F1xi1) else $
if xin le F1xi3 then F1L[j] = F1yi2+ F1k3*(xin-F1xi2) else $
if xin le F1xi4 then F1L[j] = F1yi3+ F1k4*(xin-F1xi3) else F1L[j] =
F1yi4+ F1k5*(xin-F1xi4)
;;**F2
if xin le F2xi1 then F2L[j] = F2a1+ F2k1*xin else $
if xin le F2xi2 then F2L[j] = F2yi1+ F2k2*(xin-F2xi1) else $
if xin le F2xi3 then F2L[j] = F2yi2+ F2k3*(xin-F2xi2) else $
if xin le F2xi4 then F2L[j] = F2yi3+ F2k4*(xin-F2xi3) else F2L[j] =
F2yi4+ F2k5*(xin-F2xi4)
;;**F2
if xin le PHIxi1 then PHIL[j] = PHIa1+ PHIk1*xin else $
if xin le PHIxi2 then PHIL[j] = PHIyi1+ PHIk2*(xin-PHIxi1) else $
if xin le PHIxi3 then PHIL[j] = PHIyi2+ PHIk3*(xin-PHIxi2) else $
if xin le PHIxi4 then PHIL[j] = PHIyi3+ PHIk4*(xin-PHIxi3) else
PHIL[j] = PHIyi4+ PHIk5*(xin-PHIxi4)
eF1L[j]=0.001*F1L[j];
eF2L[j]=0.001*F2L[j];
ePHIL[j]=0.001*PHIL[j];

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