Spectrometer optimisation

McStas Workshop 13th-15th April 2021

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What will we be focussing on

tof

continuou

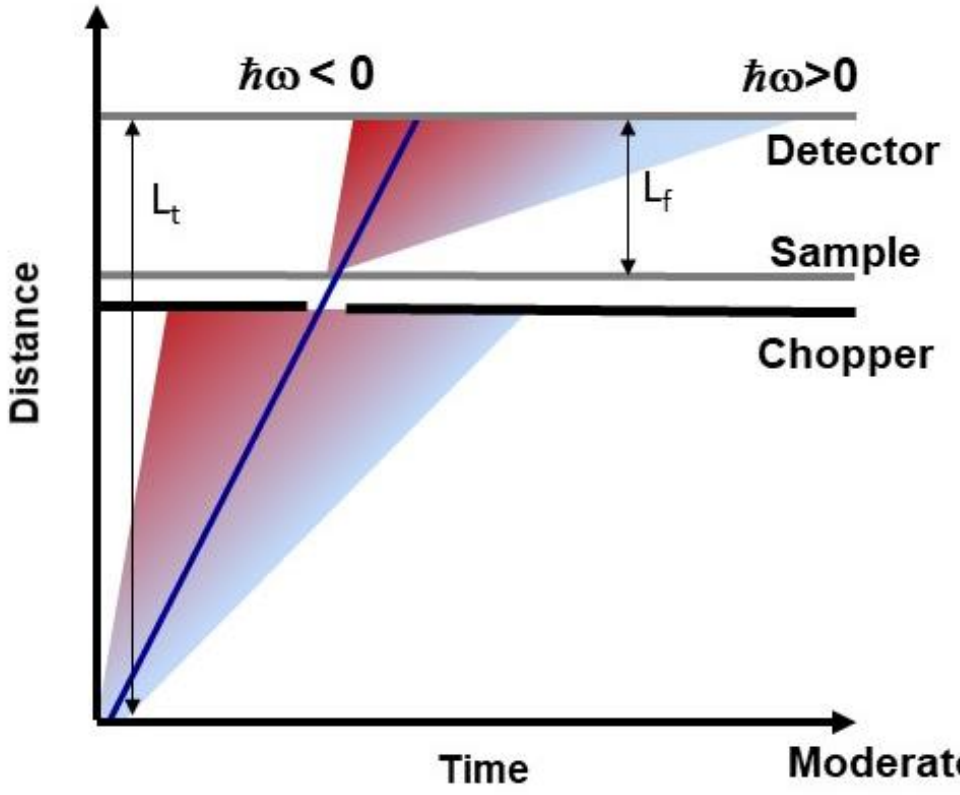
direct

in-direct

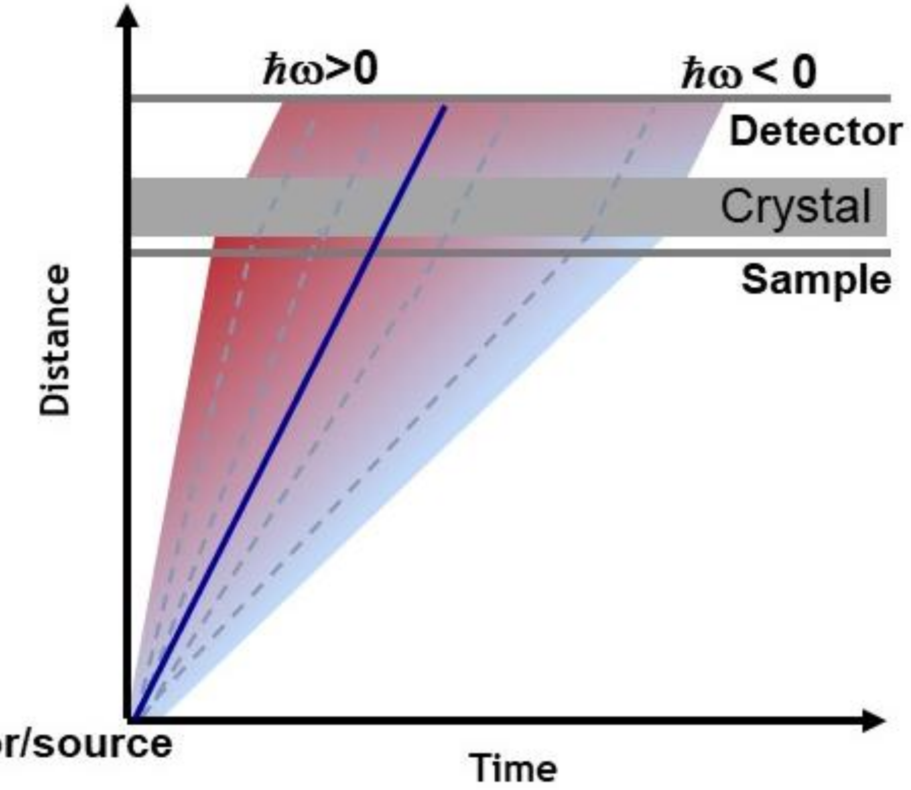
LET, IN5,MERLIN, MAPS

IRIS, TOSCA,VESUVIO

Triple a , Lagrang pin echo



Moderator/source



Where do you start designing your instrument ?

- You don’t start with McStas !!!
- Need the **key drivers** (resolution, sample environment, any limitations on design)
- Parameter space is large. To optimise its crucial to understand the ‘Maths’ of your instrument
  -how the resolution and flux depend on the instrument parameters
- What do we mean by an optimal design? – need some sort of FOM

What do we mean by an optimal design?

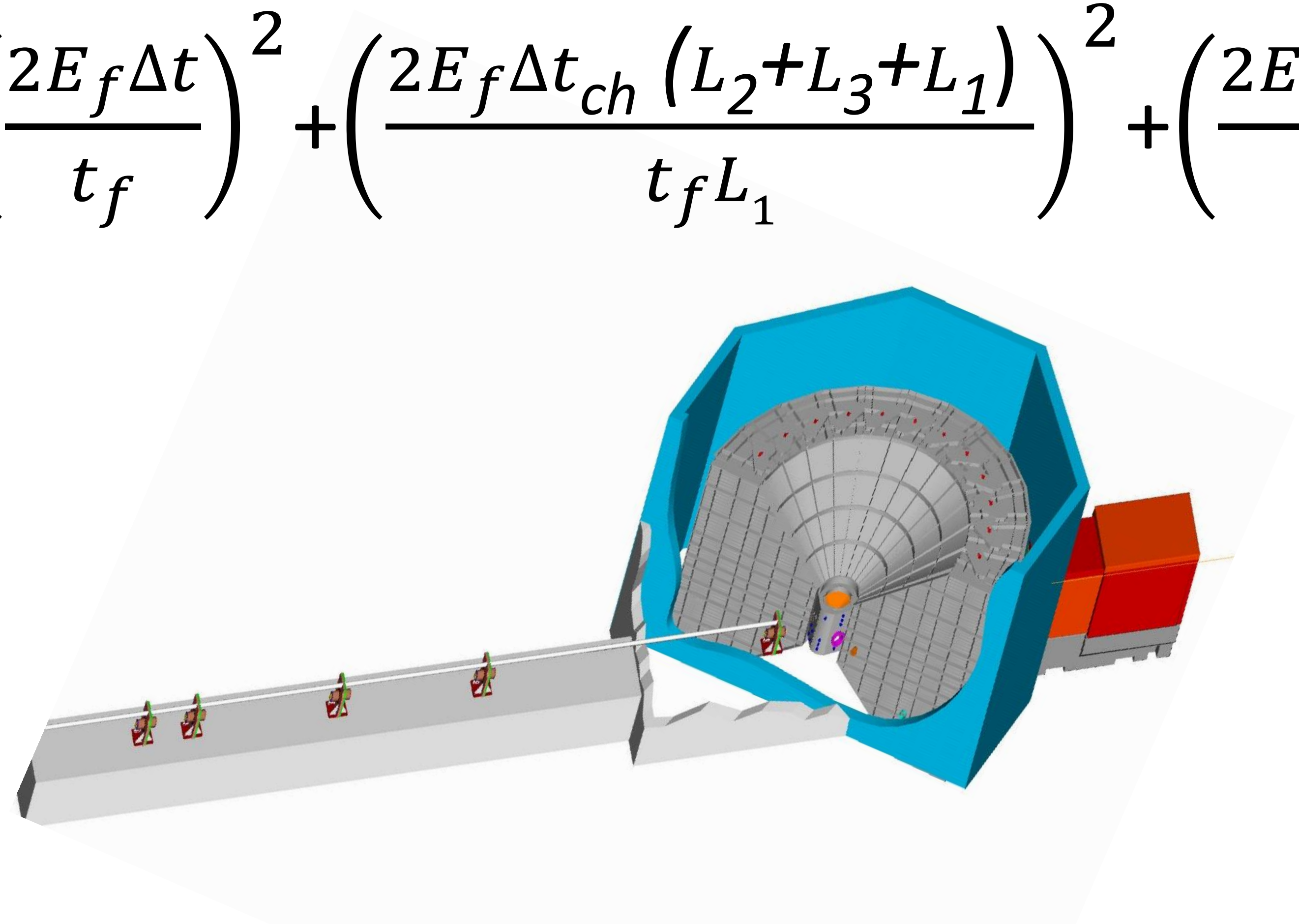
Need a Figure Of Merit

- For Engin-X FOM = $I\sigma^2/w^2$
- For spectrometers FOM = Signal/Background
- Optimal design will maximise the FOM for your key drivers
- Background Cannot really calculate or simulate. Minimise with shielding and design
- Rest of this talk is about the understanding the Maths of the instrument and how it relates to resolution and signal

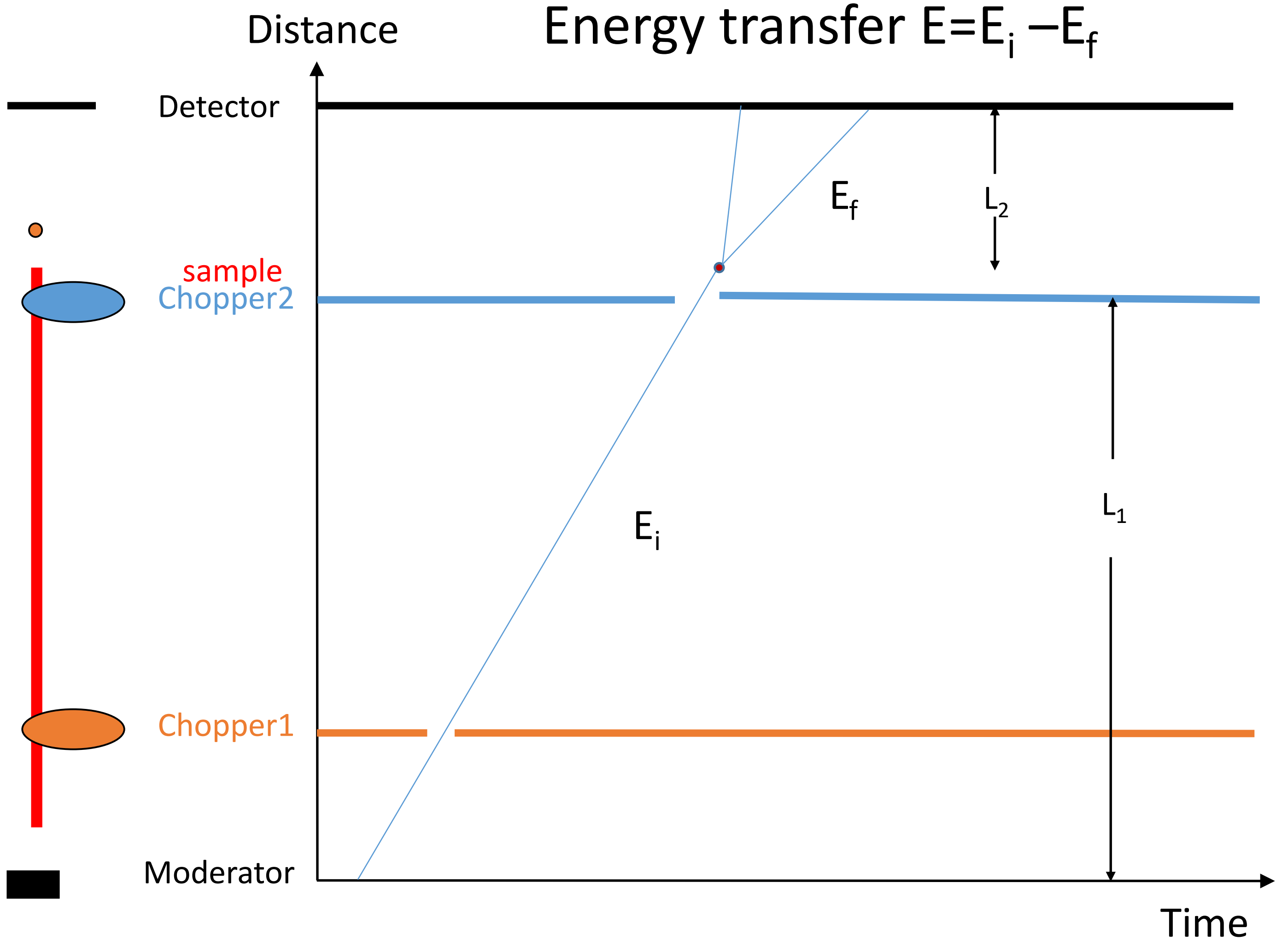
Optimising Direct TOF spectrometer (LET)

'The Maths'

$$\Delta E^2 = [\left(\frac{2E_f\Delta t}{t_f}\right)^2 + \left(\frac{2E_f\Delta t_{ch}\,(L_2+L_3+L_1)}{t_f L_1}\right)^2 + \left(\frac{2E_f\Delta t m_{od}\,L_2}{t_f L_1}\right)^2]$$



Optimising Direct TOF spectrometer (LET)



$E=E_i - E_f$ where E_i fixed

$$\frac{\Delta E}{\Delta t} = -\frac{\Delta E_f}{\Delta t}$$

Where $E_f = 1/2\, m_n (L_2/t_f)^2$

gives

?

$$\Delta E = \frac{2E_f \Delta t}{t_f}$$

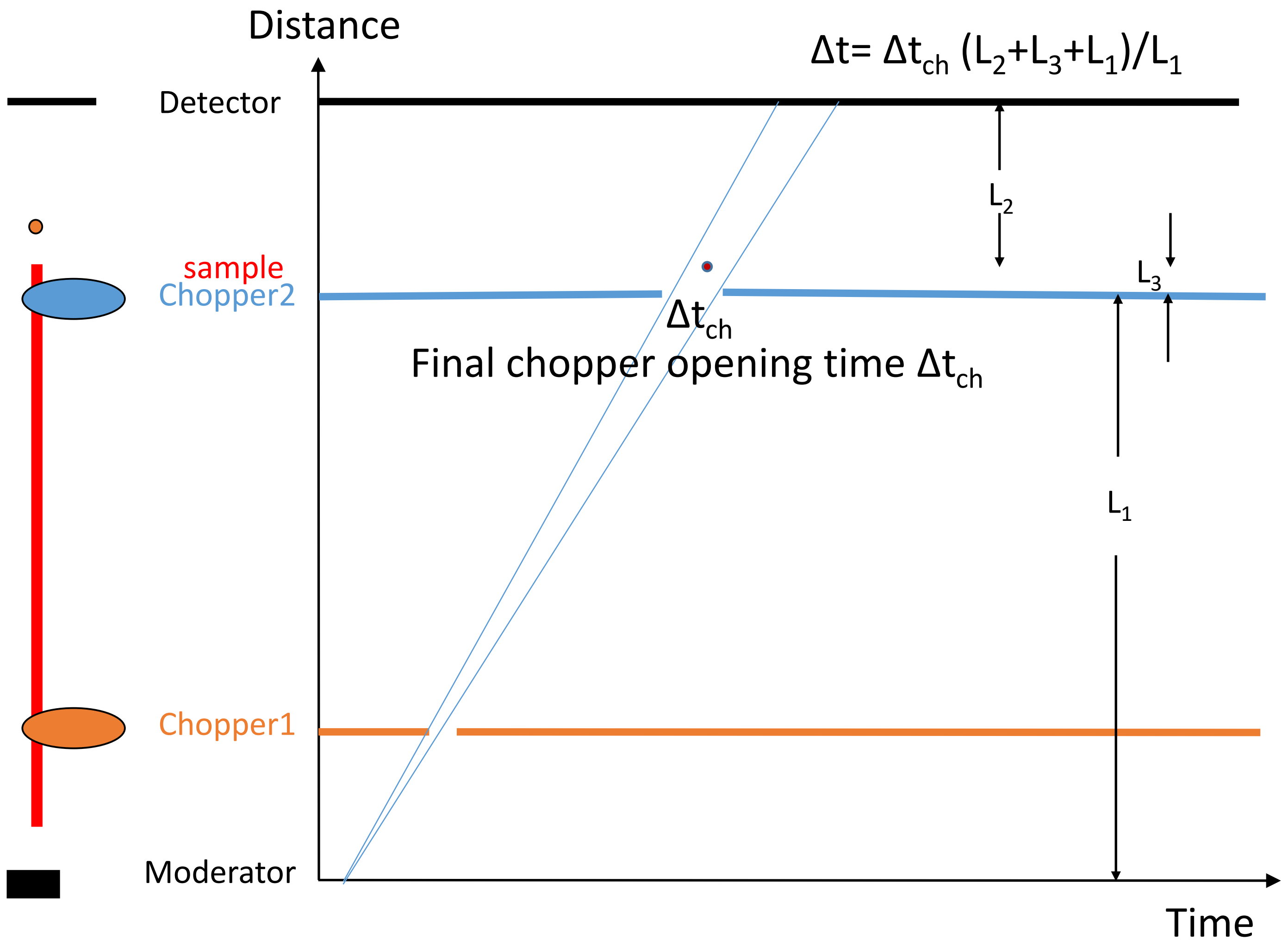
Where

ΔE	energy uncertainty
Δt	time uncertainty at detector
E_f	energy of neutron after sample
t_f	flight time sample to detector

Optimising Direct TOF spectrometer (LET)

Sources of Δt **1) Chopper opening**

$$\boxed{\Delta E = \frac{2E_f \Delta t}{t_f}}$$

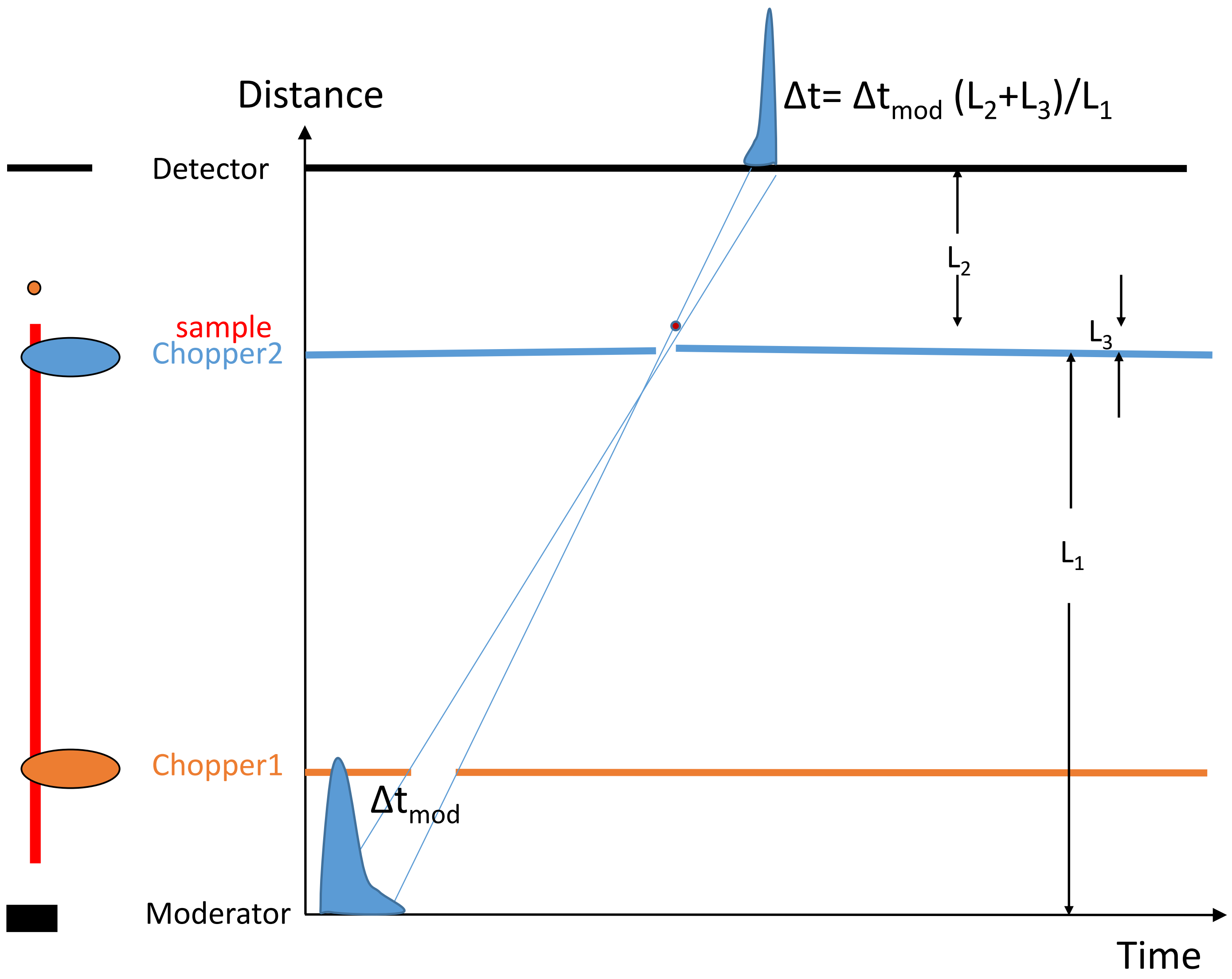


Chopper term

$$\Delta E = \frac{2E_f \Delta t c_h \left(L_2 + L_3 + L_1\right)}{t_f L_1}$$

Optimising Direct TOF spectrometer (LET)

Sources of Δt **2) Moderator**



$$\boxed{\Delta E = \frac{2E_f \Delta t}{t_f}}$$

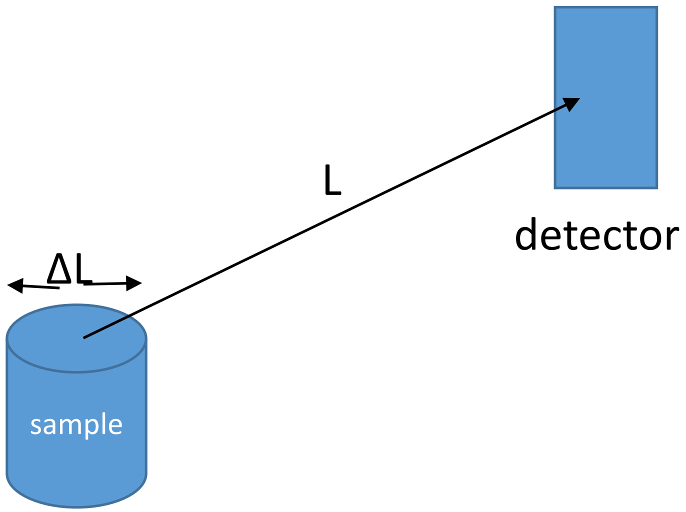
Moderator term

$$\Delta E = \frac{2E_f \Delta t m_{od}\,(L_2+L_3)}{t_f L_1}$$

Optimising Direct TOF spectrometer (LET)

Sources of Δt　　**3) Sample/detector size**

$$\Delta E = \frac{2E_f \Delta t}{t_f}$$



$$\frac{\Delta t}{t_f} = \frac{\Delta L}{L}$$

On LET　ΔL =2 cm and L =350 cm (sample to detector distance)

$$\frac{\Delta E}{E_f} = \frac{2x2}{350} \approx 1\%$$

- Sample size only significant when energy resolution is close to 1%

Optimising Direct TOF spectrometer (LET)

Assuming no correlations all the terms convolute together. A good approximation is to add in quadrature

$$\Delta E^2 = \Delta E^2_{sam} + \Delta E^2_{chop} + \Delta E^2_{mod}$$

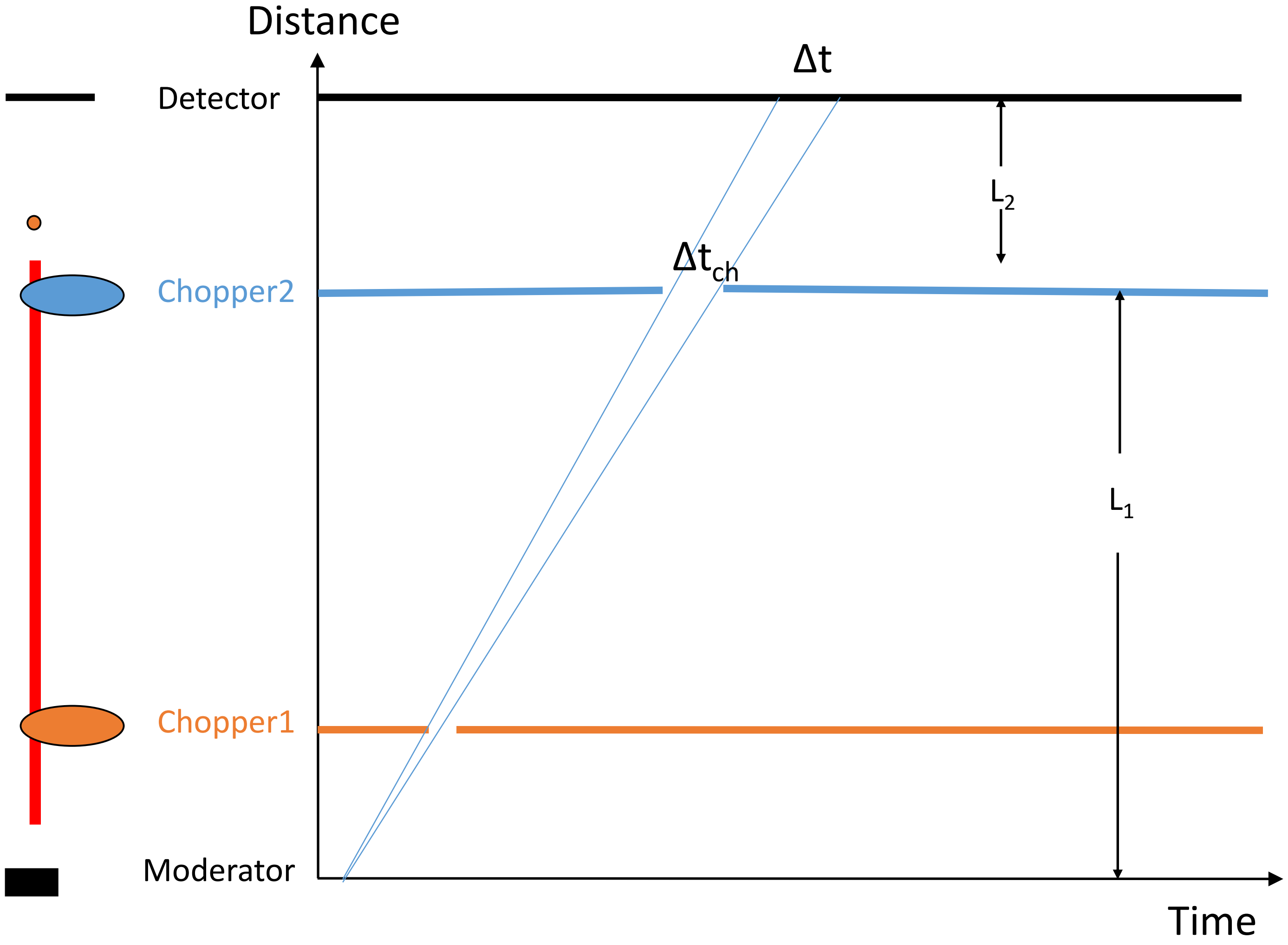
sample chopper moderator

$$\Delta E^2 = \left[\left(\frac{2E_f \Delta t_{sam}}{t_f}\right)^2 + \left(\frac{2E_f \Delta t_{chop}\,(L_2+L_3+L_1)}{t_f L_1}\right)^2 + \left(\frac{2E_f \Delta t m_{od}\, L_2}{t_f L_1}\right)^2\right]$$

What does it all mean?

Optimising Direct TOF spectrometer (LET)
Optimising L_2

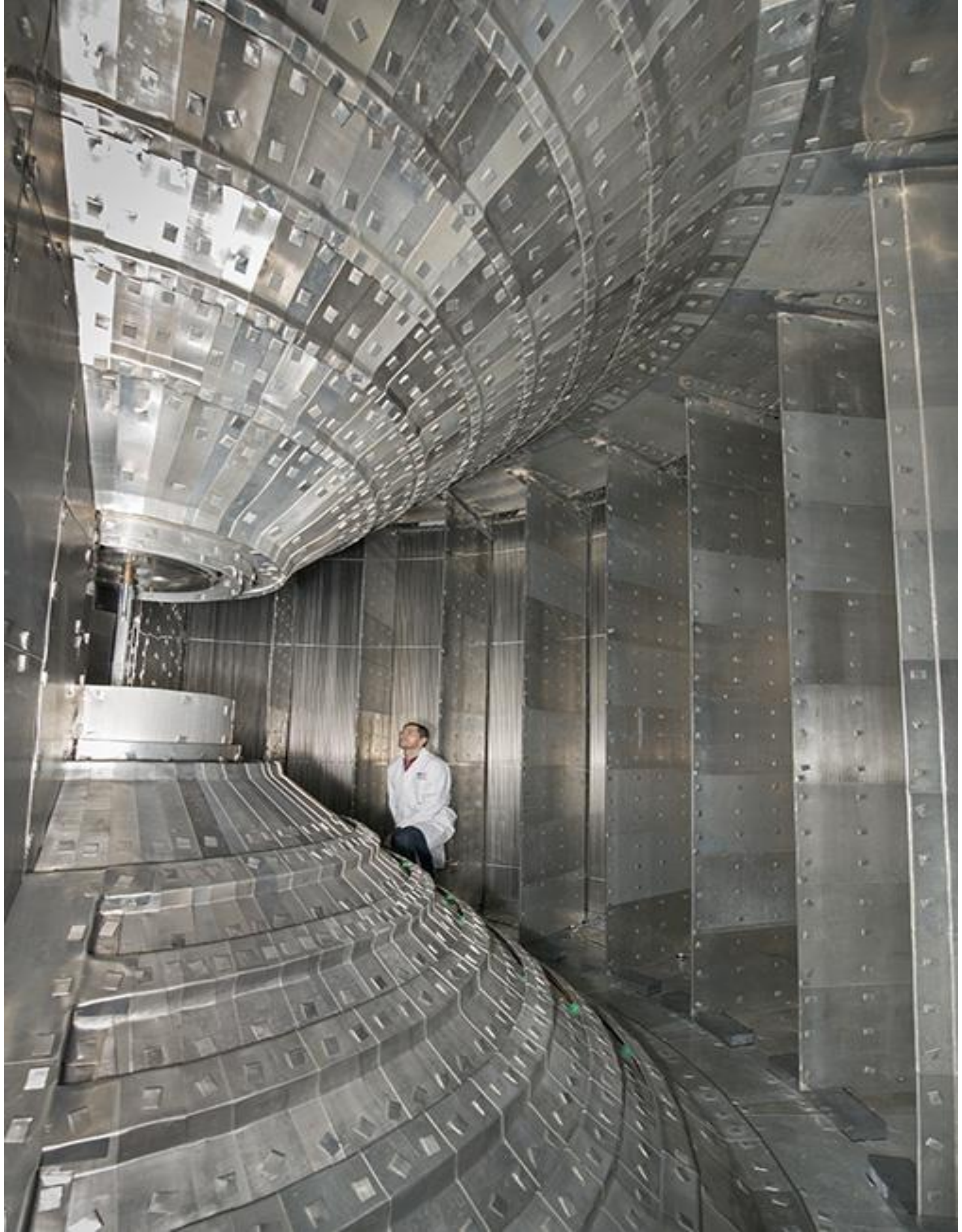
$$\Delta E = \frac{2E_f \Delta t}{t_f}$$



$$\Delta E = \frac{2E_f \Delta t}{252.8\lambda_f L_2}$$

- Better resolution with larger L_2
- For fixed ΔE count rate goes as L_2

- Make L_2 as large as possible
- Gives better resolution
- Gives larger count rate
- Remember cost goes as L_2^2

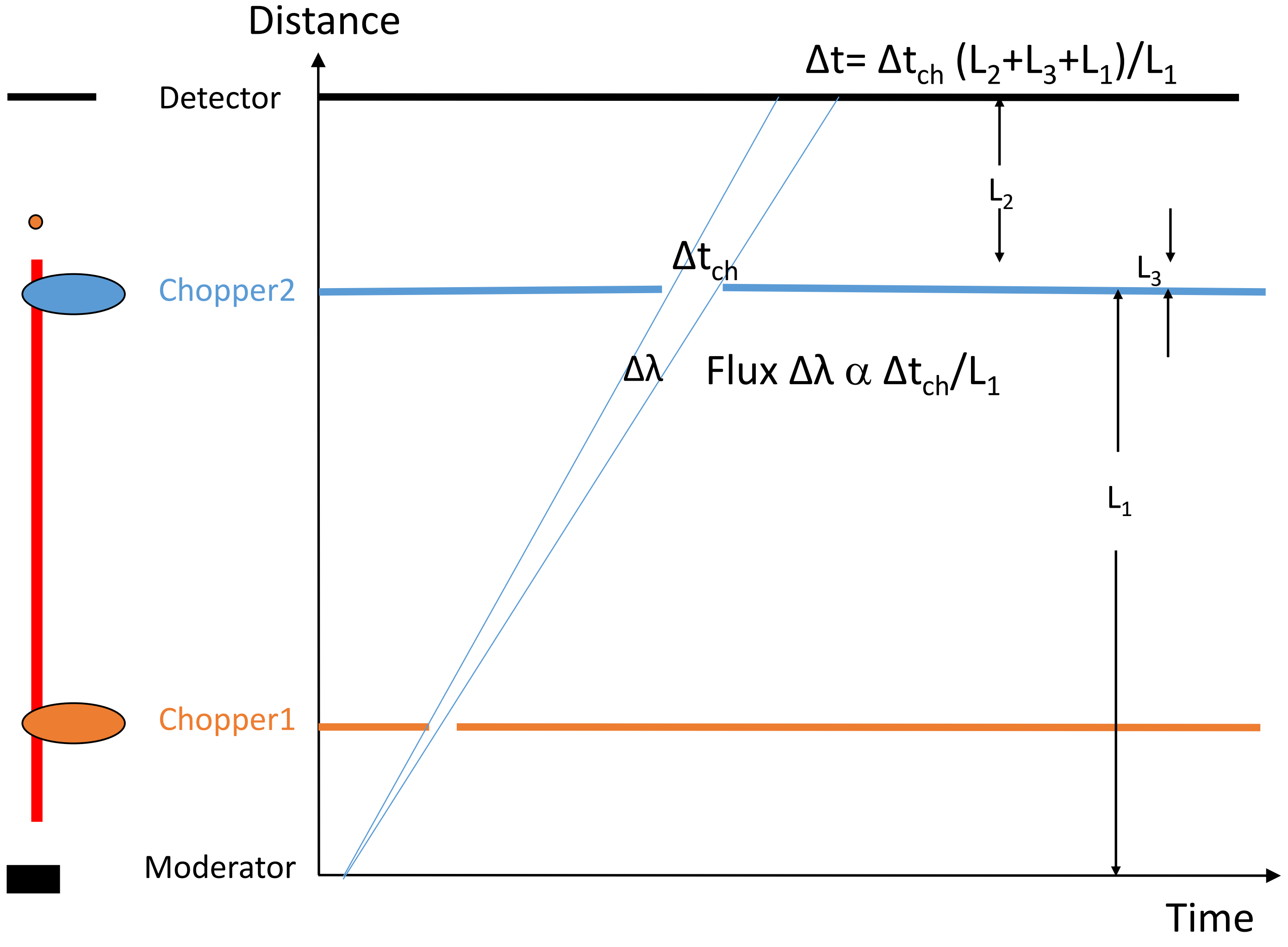


- Main cost of Direct geometry spectrometers from secondary
- LET has 40 m^2 of detectors (approx. £20M today)

Optimising Direct TOF spectrometer (LET)

Optimising L_1

$$\Delta E = \frac{2E_f \Delta t}{t_f}$$

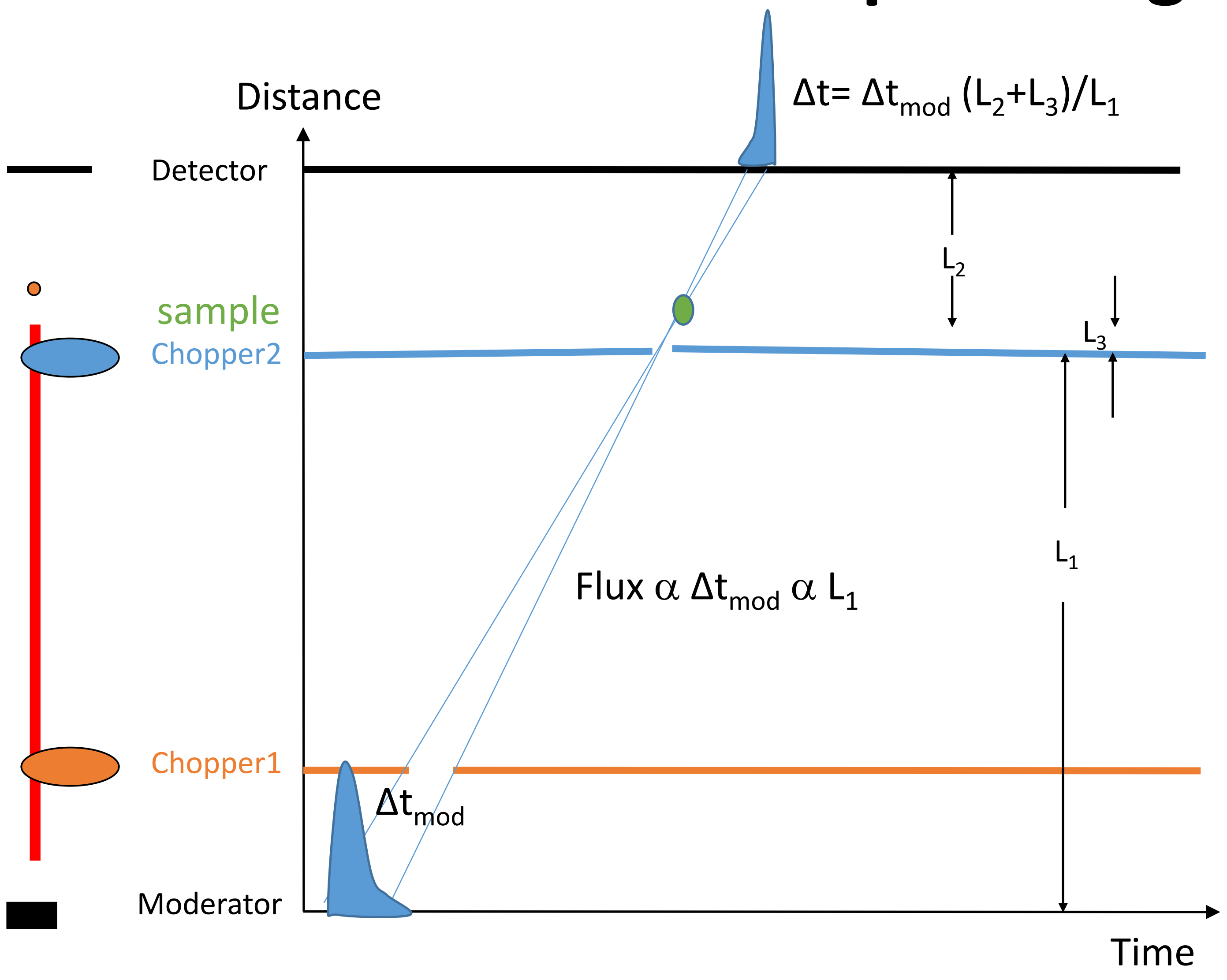


- keep ΔE constant just vary L_1
- So Δt L_2, L_3 are kept constant
- Flux α $\Delta t_{ch}/L_1 = \Delta t/(L_2+L_3+L_1)$
- Flux α $1/(a+L_1)$ where $(a=L_2+L_3)$
- When $L_1 >> L_2+L_3$
- flux ≈ α $1/L_1$ for constant ΔE

Make L_1 as short as possible ????

Optimising Direct TOF spectrometer (LET)

Optimising L_1



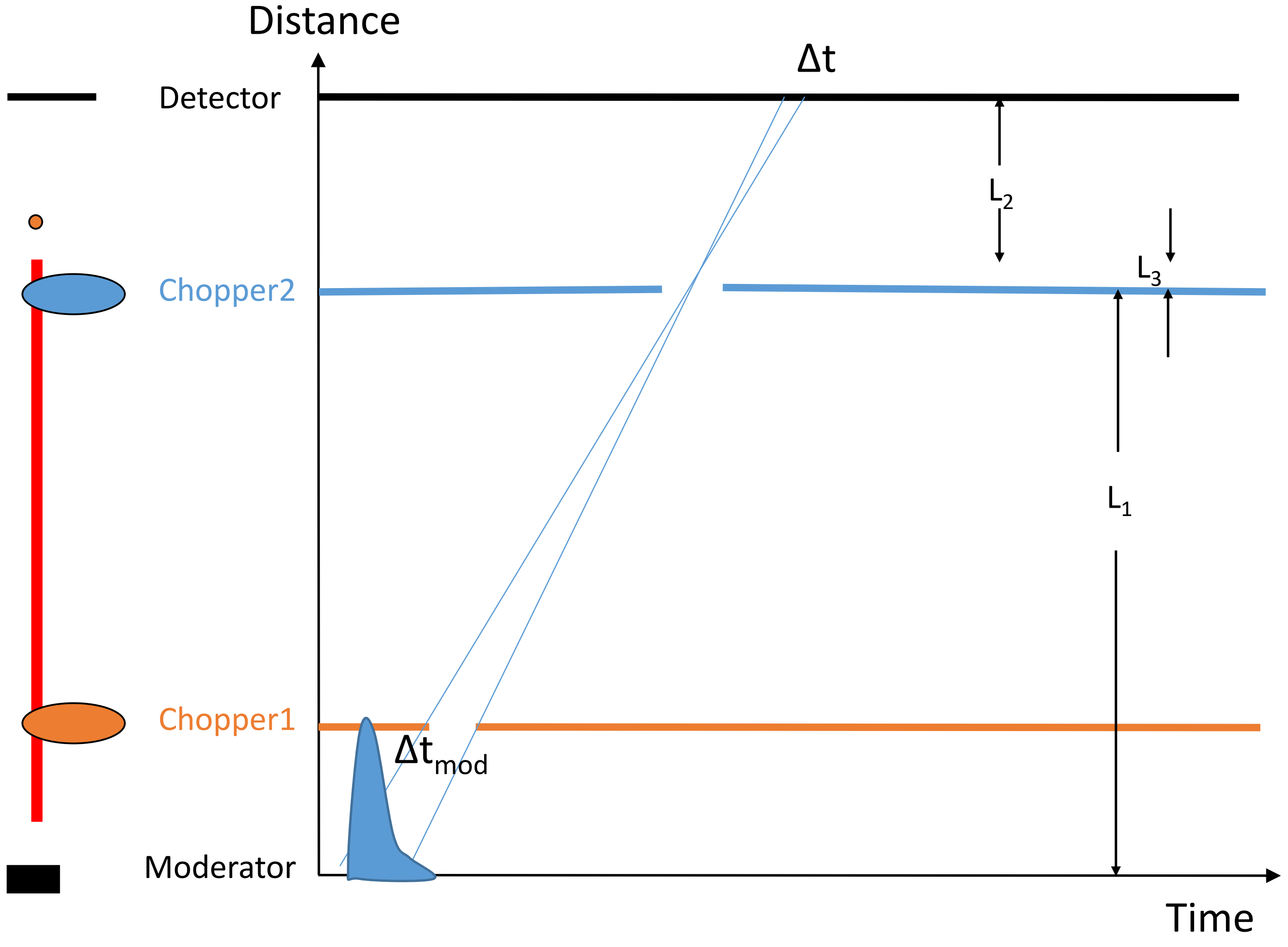
$$\Delta E = \frac{2E_f \Delta t}{t_f}$$

- keep ΔE constant just vary L_1
- So Δt L_2, L_3 are kept constant
- flux α $\Delta t_{mod} = L_1 \Delta t/ (L_2+L_3)$
- flux α L_1

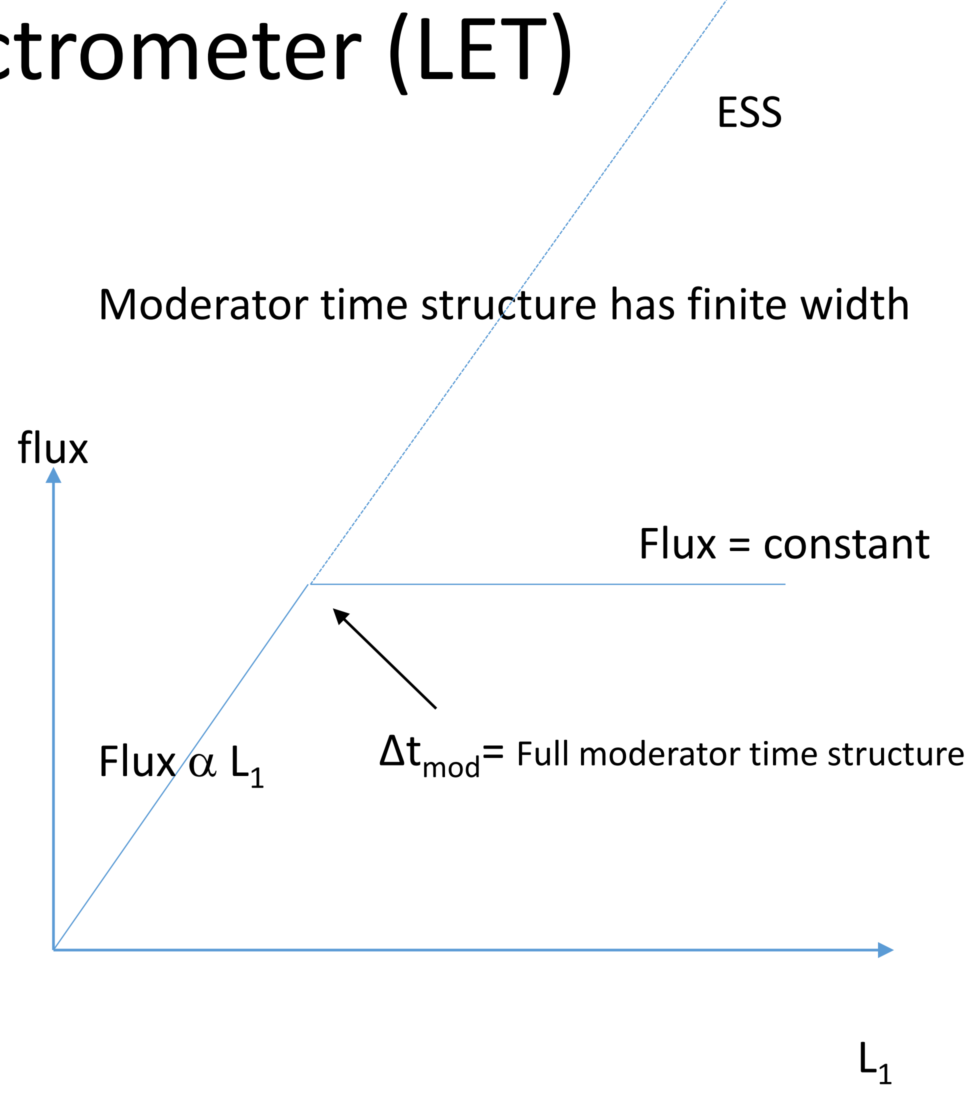
So flux increases with L_1 ???

Optimising Direct TOF spectrometer (LET)

Optimising L_1



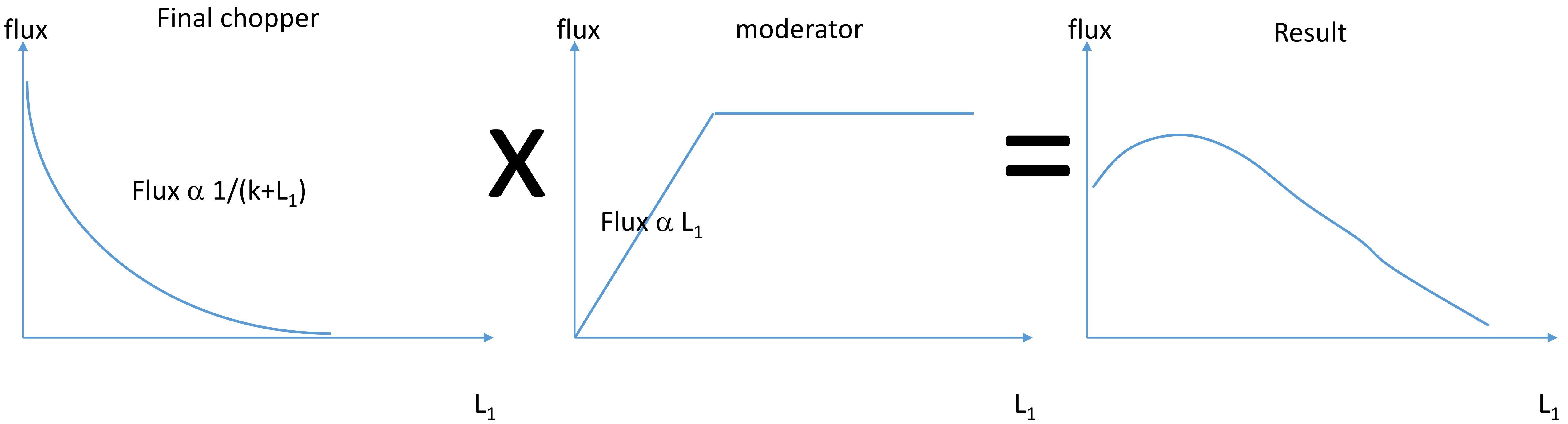
Moderator time structure has finite width



Optimising Direct TOF spectrometer (LET)

Optimising L_1

Total flux is chopper term x moderator term

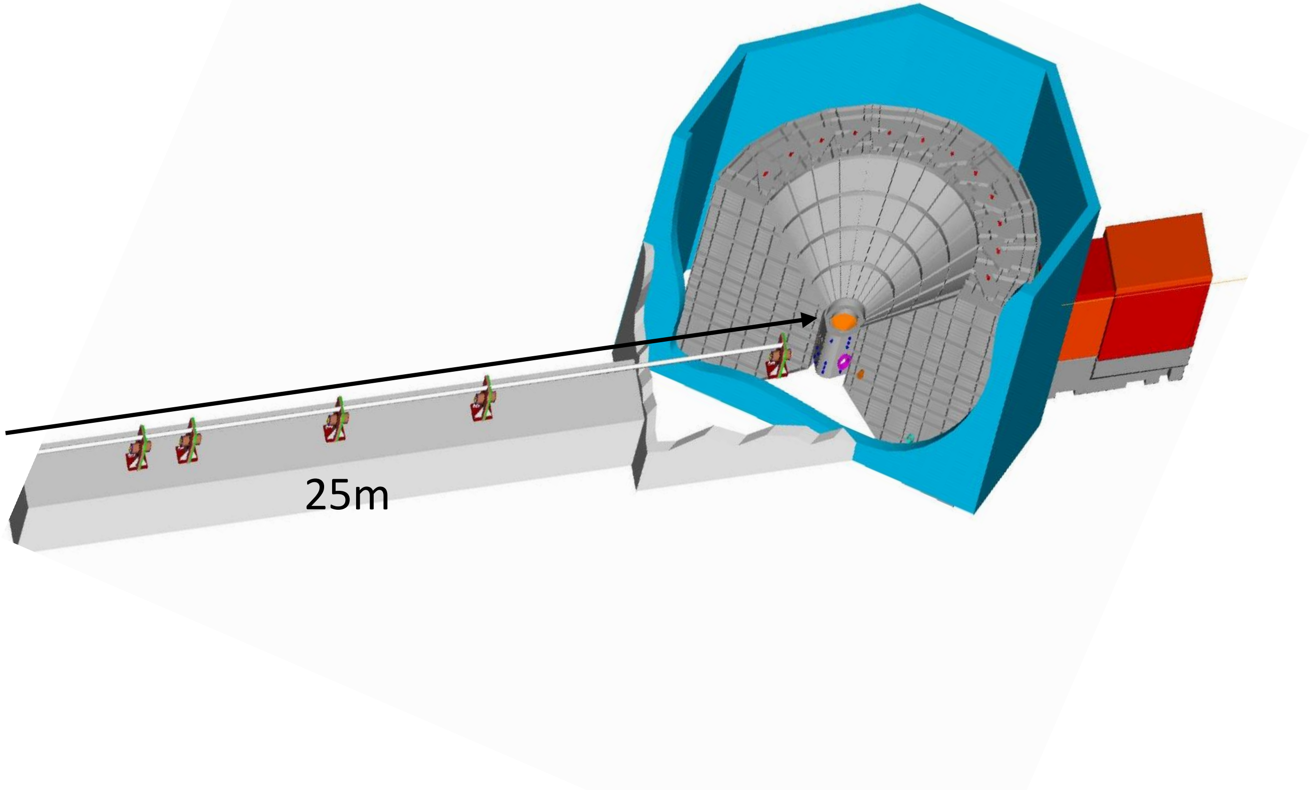


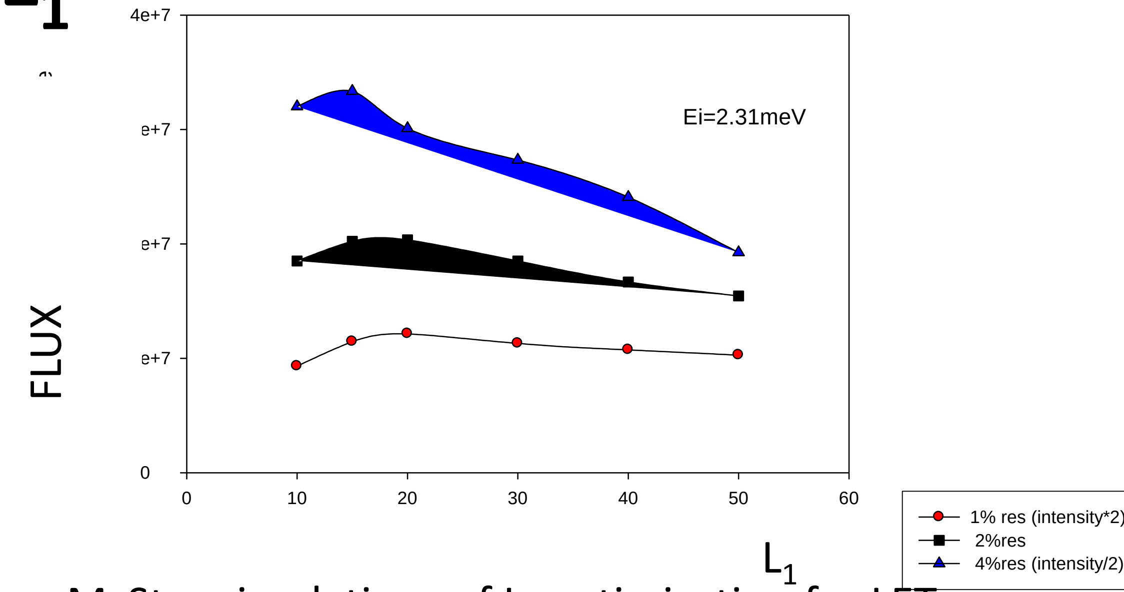
N.B This is nothing to do with guides. It's a consequence of the resolution equations

Optimising Direct TOF spectrometer (LET)

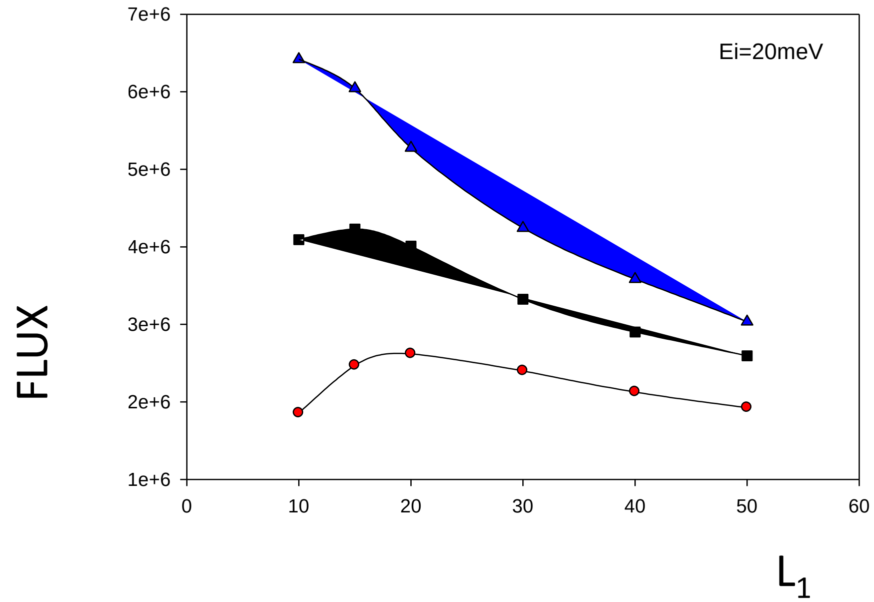
Optimising L_1

- Optimal L_1 is slightly less than 20m
- For LET set L_1=25m as need space for detectors





McStas simulations of L_1 optimisation for LET

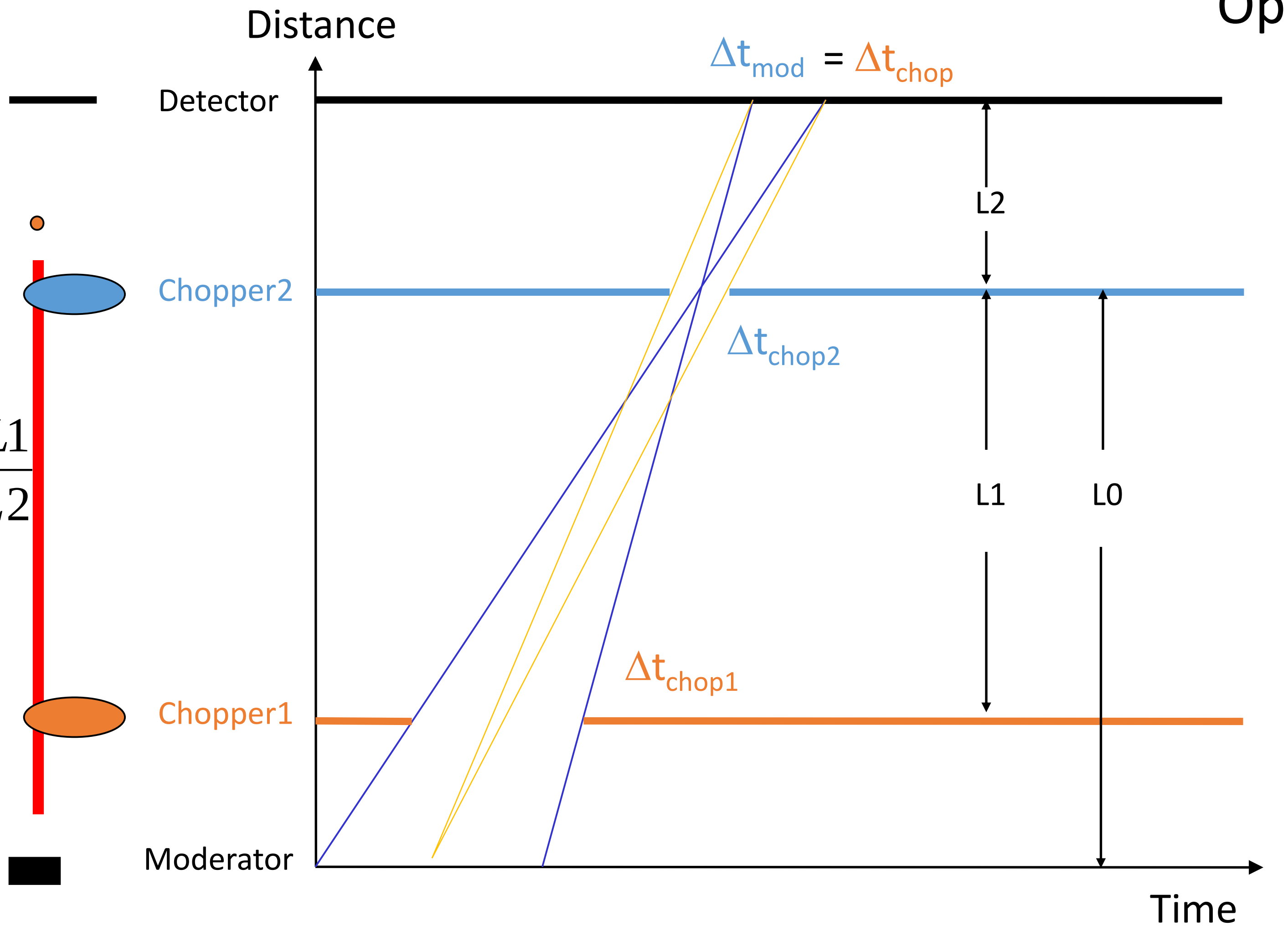


Optimising Direct TOF spectrometer (LET)

Optimising chopper openings

Optimization condition

$$\frac{\Delta t_{chop1}}{\Delta t_{chop2}} = \frac{L2 + L0}{L0}\,\frac{L1}{L2}$$



Optimise count rate by setting

$\Delta t_{mod} = \Delta t_{chop}$

The rule is

$\Delta t_{chop} => \Delta t_{mod}$

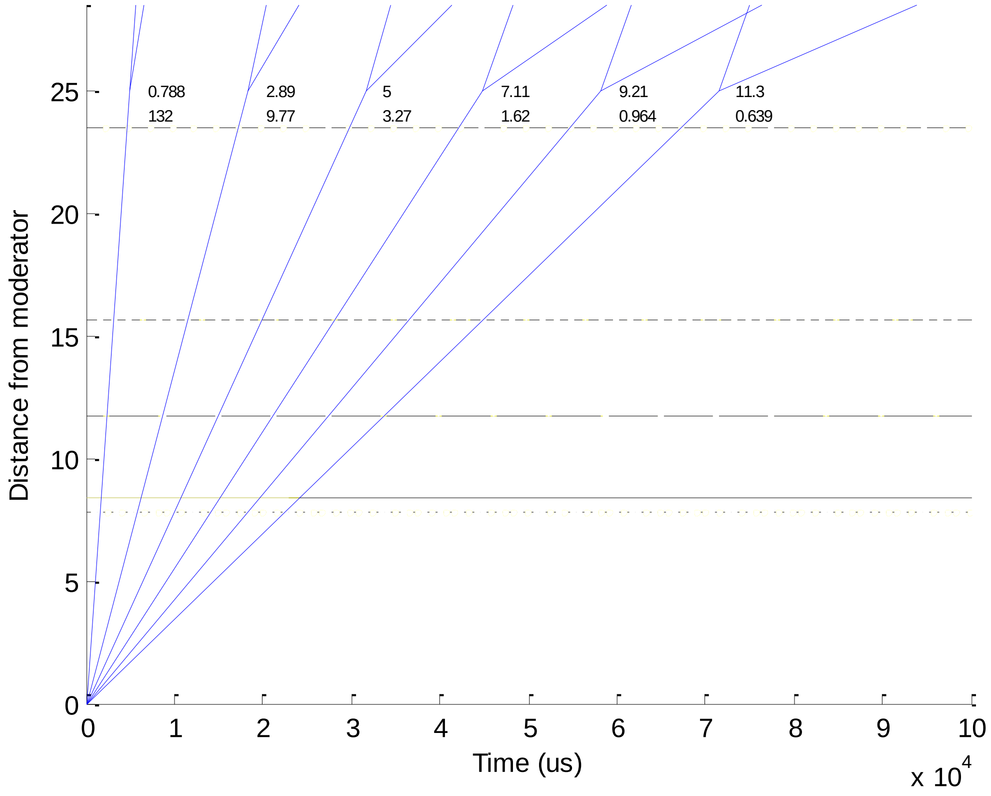
Optimising Direct TOF spectrometer (LET)

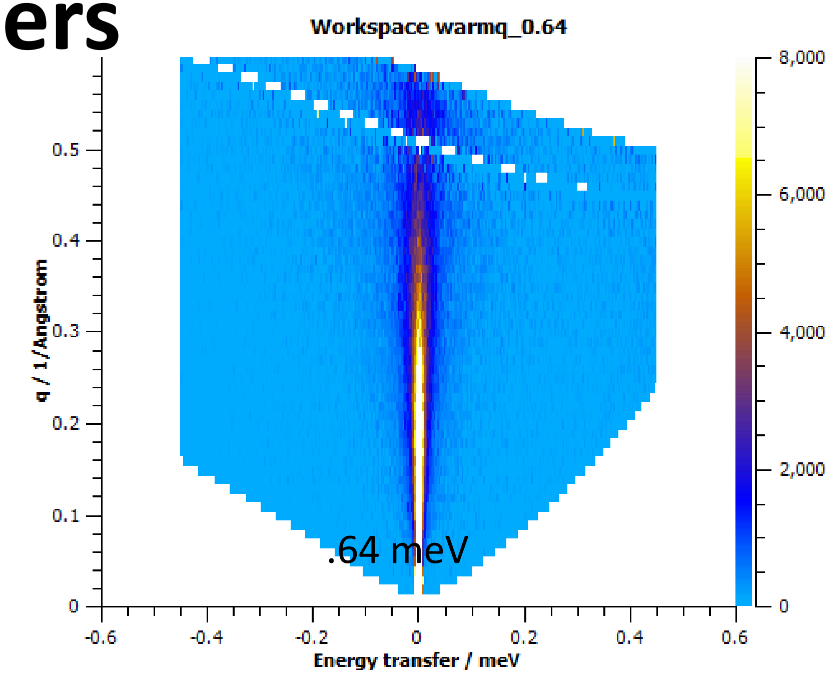
Optimising choppers

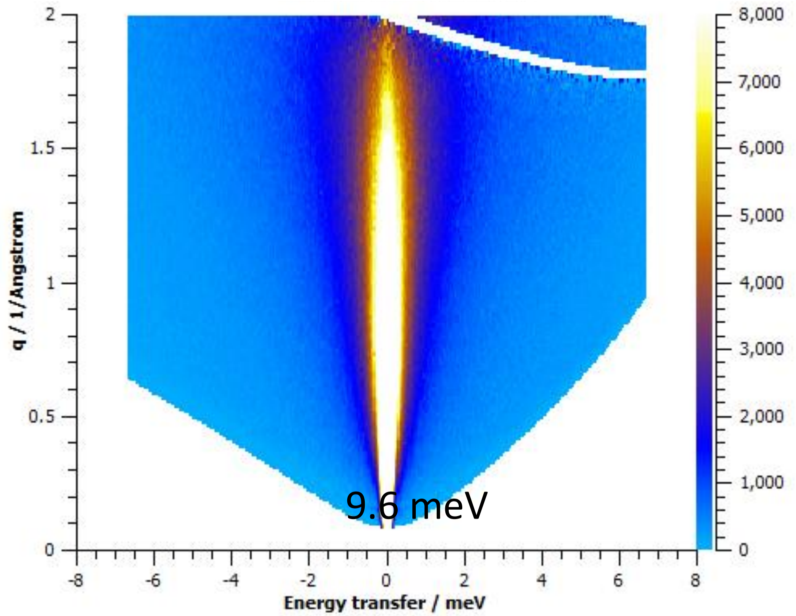
- Single measurement use fraction of time frame

- LET has a special chopper arrangement allowing multiple E_i

9.6 3.3 1.6 .96 .64 mev







Optimising Direct TOF spectrometer (LET)

SUMMARY

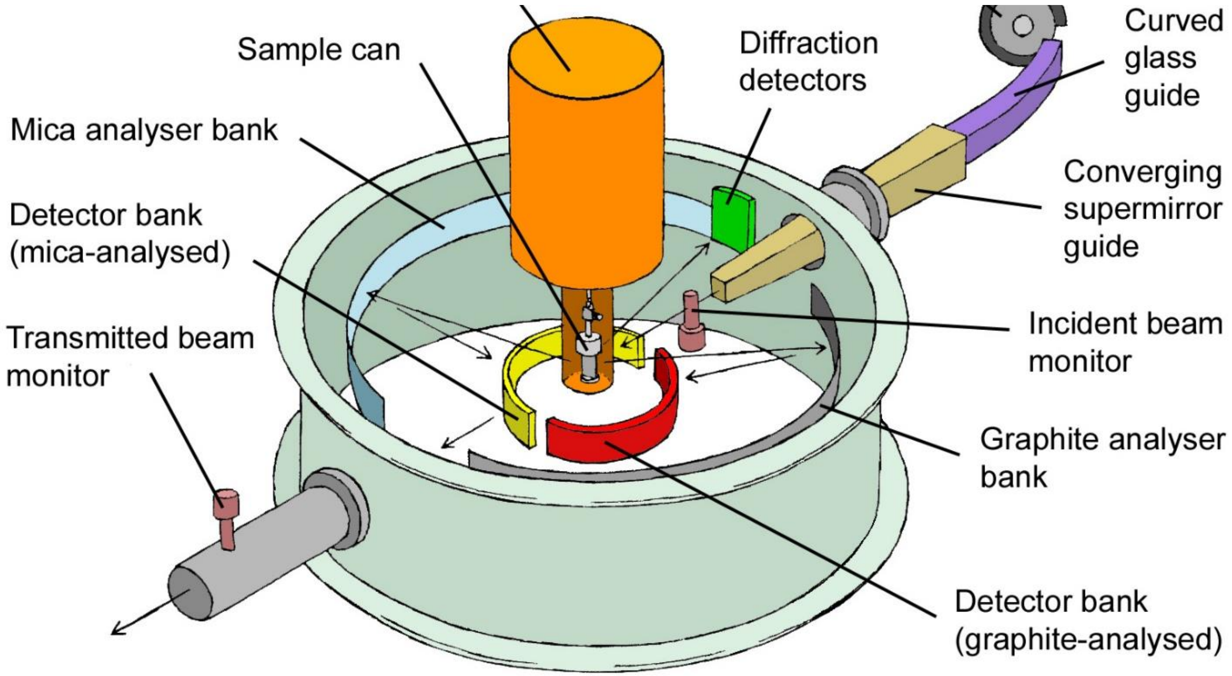
RULES to maximise your signal

- Make L2 as large as possible (better resolution and flux)
- There is an optimal L1
- Match moderator and chopper terms $\Delta E_{mod} = \Delta E_{chop}$ when possible
- Include RRM to fill the time frame

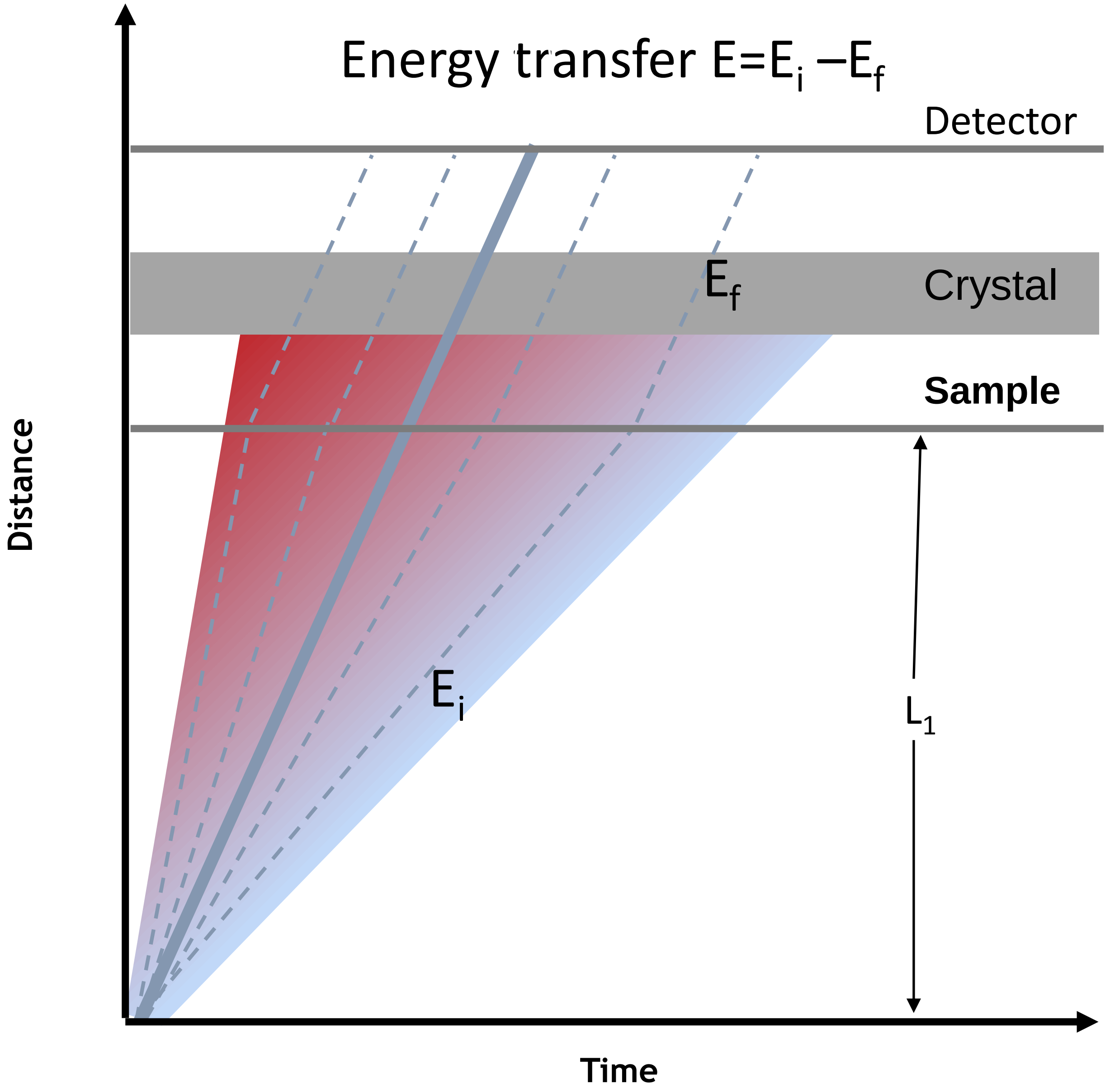
Optimising an In-direct TOF spectrometer (IRIS)

‘The Maths’

$$\Delta E^2 = \left[\left(\frac{2E_i\Delta t_{sam}}{t_i}\right)^2 + \left(2\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)\left(\frac{t_f E_i}{t_i} + E_f\right)\right)^2 + \left(\frac{2E_i\Delta t m_{od}}{t_i}\right)^2\right]$$



Optimising an Indirect TOF spectrometer (IRIS)



$E = E_i - E_f$ where E_f fixed

$$\frac{\Delta E}{\Delta t} = -\frac{\Delta E_i}{\Delta t}$$

Where $E_i = \frac{1}{2} m_n (L_1/t_i)^2$

?

$$\boxed{\Delta E = \frac{2E_i \Delta t}{t_i}}$$

ΔE	energy uncertainty
Δt	time uncertainty at detector
E_i	energy of neutron on sample
t_i	flight time moderator to sample

Comparison In-direct v direct

In-direct

$$\Delta E = \boxed{\frac{2E_i \Delta t}{t_i}}$$

Direct

$$\Delta E = \boxed{\frac{2E_f \Delta t}{t_f}}$$

$t_i >> t_f$ so ΔE smaller on In-direct for same Δt (In-direct for high resolution)

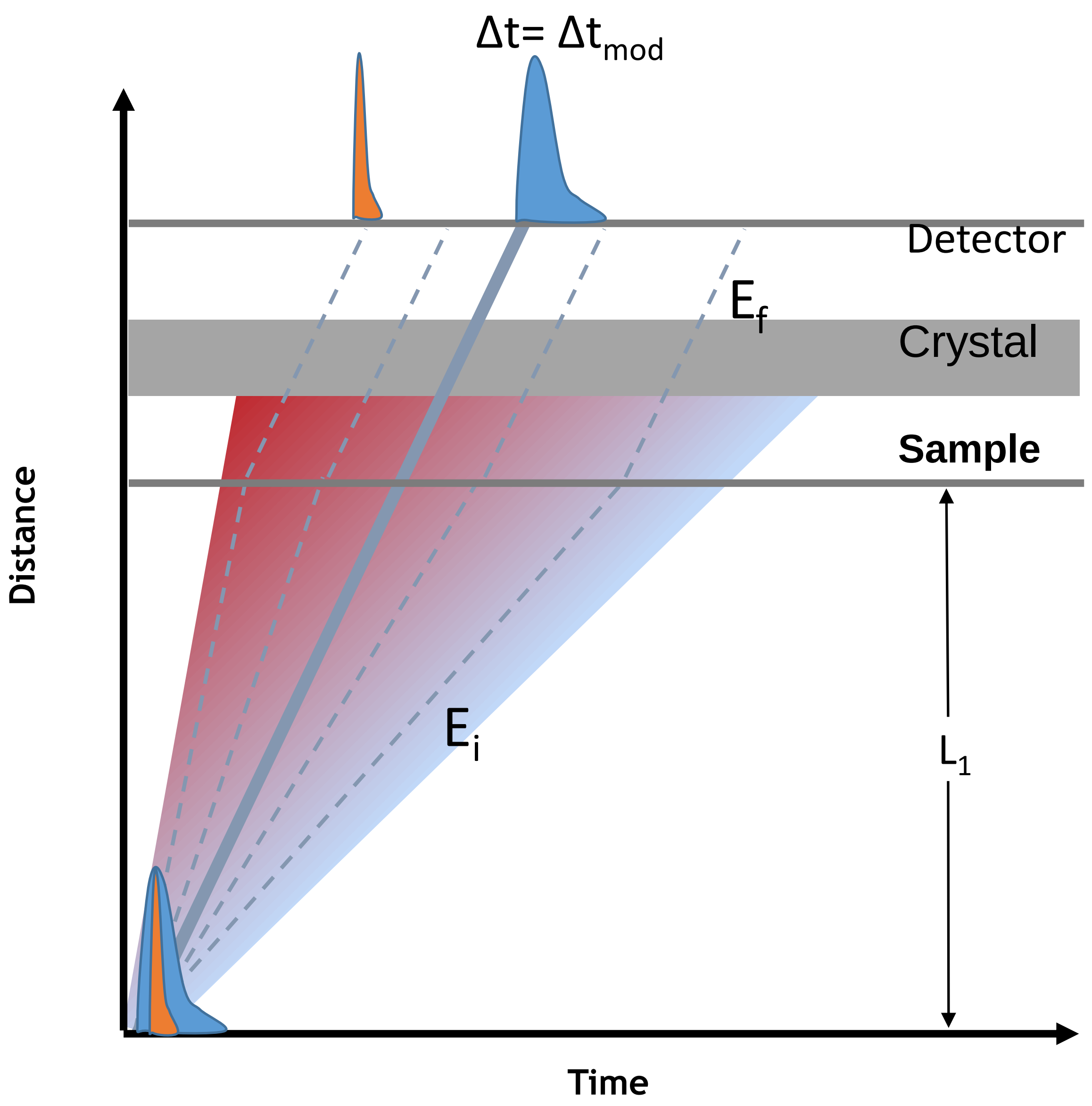
OR

For same ΔE can accept larger Δt and hence more flux (In-direct for higher count rate)

Optimising an Indirect TOF spectrometer (IRIS)

Sources of Δt **1) Moderator**

$$\Delta E = \frac{2E_i \Delta t}{t_i}$$



- Δt_{mod} doesn't alter from moderator to detector

$$\Delta E = \frac{2E_i \Delta tm_{od}}{t_i}$$

RESOLUTION

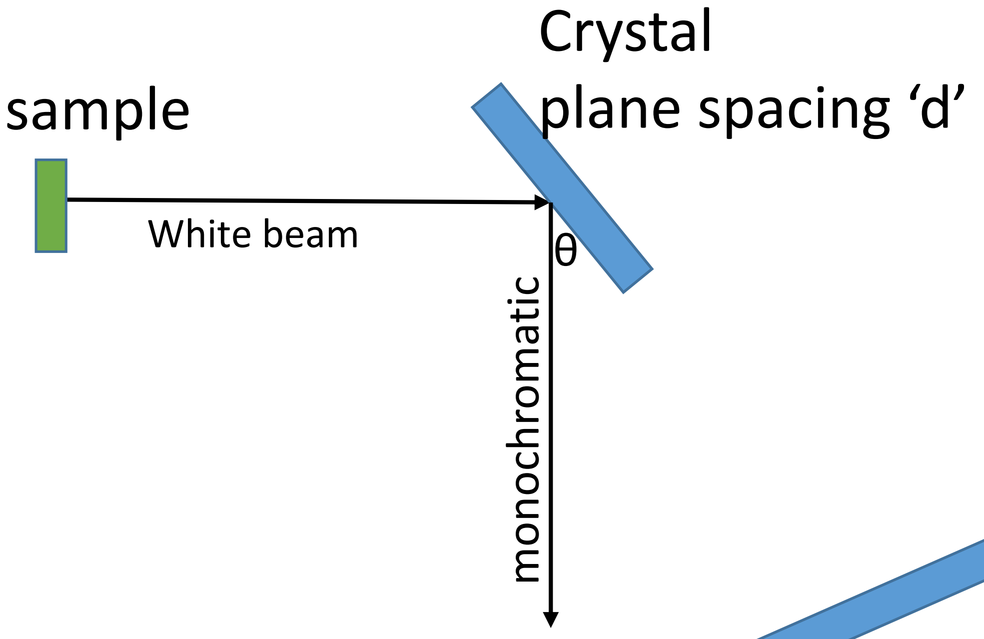
- Increasing L_1 reduces contribution of Δt_{mod} on ΔE

FLUX

- Flux α Δt_{mod} but is independent of L_1 or L_2

Optimising an Indirect TOF spectrometer (IRIS)

Sources of Δt 2) Analyser Crystal



$\lambda_f = 2d\sin\theta$

Differentiating Braggs law gives

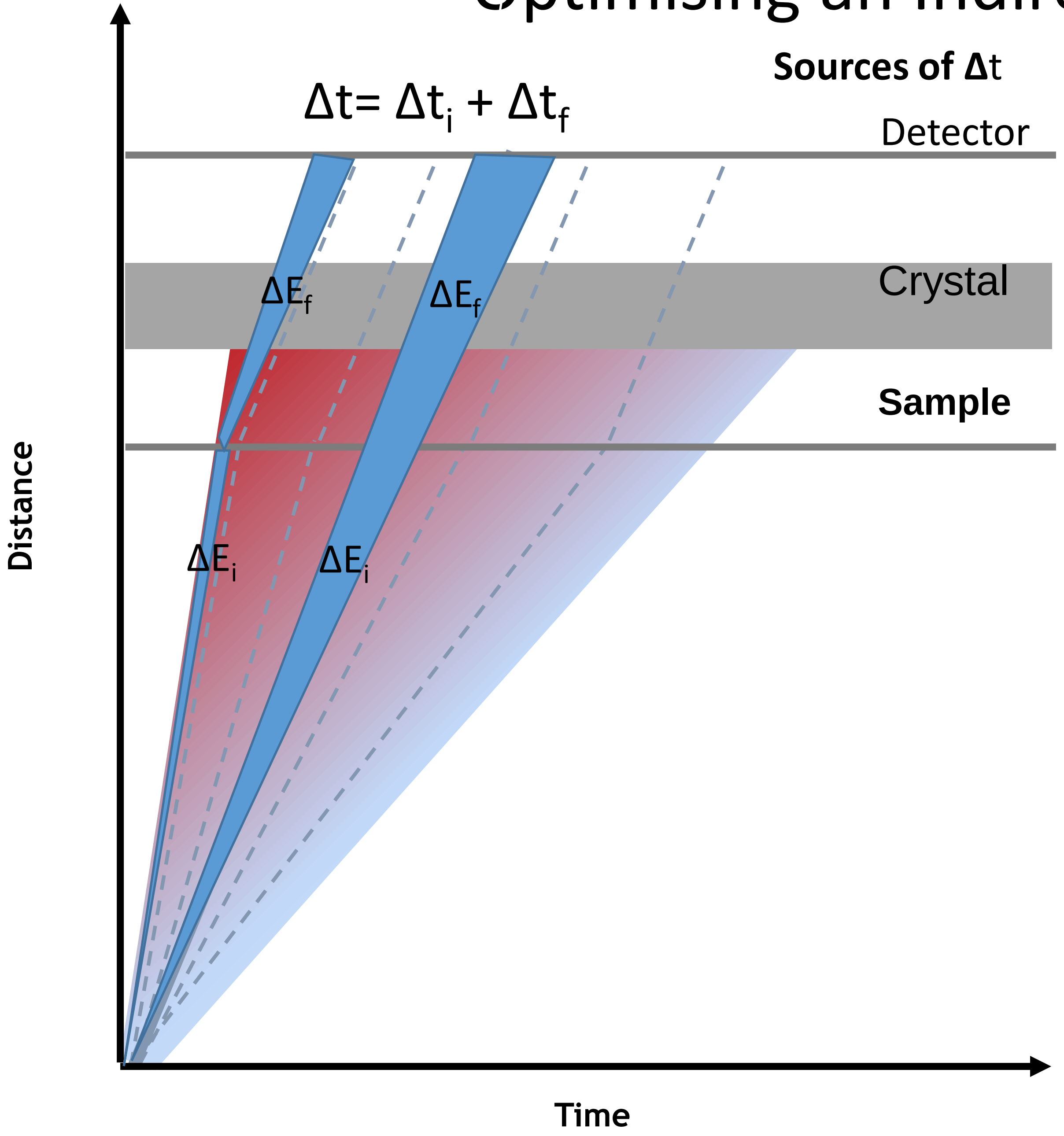
$$\frac{\Delta\lambda_f}{\lambda_f} = \frac{\Delta d}{d} + \cot\theta\Delta\theta$$

Δλ is wavelength spread
Δd is spread in d spacing
Θ is Bragg angle
ΔΘ Bragg angle spread (mosaic + sample size)

$$\frac{\Delta E}{E} = \frac{2\Delta\lambda}{\lambda} \qquad \text{thus} \quad \Delta E_f = 2E_f\left(\frac{\Delta d}{d} + \cot\theta\Delta\theta\right)$$

ΔE_f is the energy spread of neutrons coming off the analyser

Optimising an Indirect TOF spectrometer (IRIS)



2) Analyser Crystal

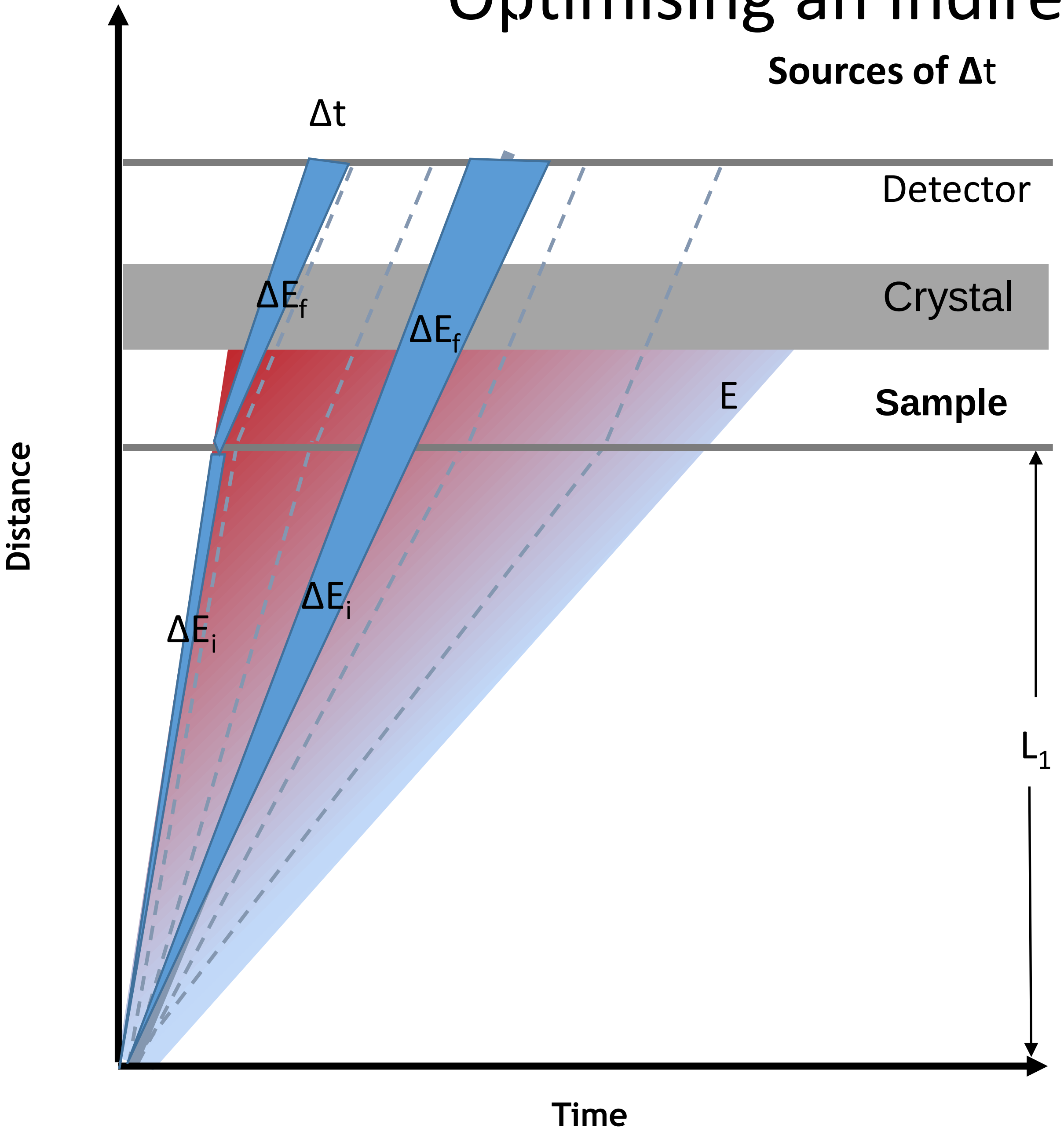
$$\Delta E = \frac{2E_i \Delta t}{t_i}$$

- 1) $\Delta E_f = 2E_f\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)$ is a constant
- 2) Or $\Delta t_f = t_f\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)$
- 3) BUT $\Delta E_i = \Delta E_f$ for any constant energy transfer
- 4) gives $\Delta t_i = t_i \frac{E_f}{E_i}\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)$ from 1) and 3)
- 5) $\Delta t = \Delta t_i + \Delta t_f$
- Thus $\Delta t = \left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)\left(t_i \frac{E_f}{E_i} + tf\right)$ from2) and 4)
- Or $\boxed{\Delta E = 2\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)\left(\frac{t_f E_i}{t_i} + E_f\right)}$

Optimising an Indirect TOF spectrometer (IRIS)

Sources of Δt **2) Analyser Crystal**

$$\Delta E = \frac{2E_i \Delta t}{t_i}$$



RESOLUTION

- $\Delta E = 2\left(\frac{\Delta d}{d} + \cot\theta\Delta\theta\right)\left(\frac{t_f E_i}{t_i} + E_f\right)$
- As $\theta \rightarrow 90$ $\cot\theta\Delta\theta \rightarrow 0$ minimise ΔE

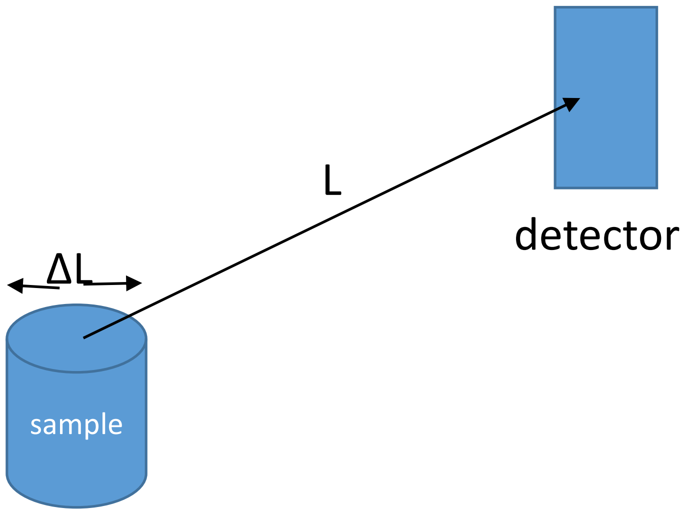
FLUX

- Flux α $\Delta E_f = 2E_f\left(\frac{\Delta d}{d} + \cot\theta\Delta\theta\right)$
- Increase flux with decreasing θ but independent of L_1 and L_2

Optimising an Indirect TOF spectrometer (IRIS)

Sources of Δt 3) Sample/detector size

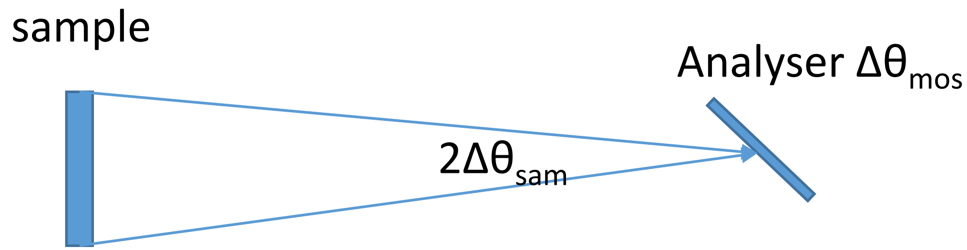
$$\Delta E = \frac{2E_i \Delta t}{t_i}$$



$$\Delta E = \frac{2E_i \Delta t s_{am}}{t_i}$$

Where $\frac{\Delta t_{sam}}{t_f} = \frac{\Delta L}{L}$

More important is the angular uncertainty from sample size $\Delta\theta_{sam}$



The total uncertainty $\Delta\theta^2 = \Delta\theta^2_{sam} + \Delta\theta^2_{mos}$

Optimising an Indirect TOF spectrometer (IRIS)

Assuming no correlations all the terms convolute together. A good approximation is to add in quadrature

$$\Delta E^2 = \Delta E^2_{sam} + \Delta E^2_{ana} + \Delta E^2_{mod}$$

sample analyser moderator

$$\Delta E^2 = \left[\left(\frac{2E_i \Delta t_{sam}}{t_i}\right)^2 + \left(2\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)\left(\frac{t_f E_i}{t_i} + E_f\right)\right)^2 + \left(\frac{2E_i \Delta tmod}{t_i}\right)^2\right]$$

Optimising an Indirect TOF spectrometer (IRIS)

Summary

- Flux from moderator or analyser does not depend on L1 or L2
- Only thing changing flux is energy spread accepted by analyser $\Delta E = E \cot\theta\Delta\theta$
- Flux increases as Bragg angle θ reduces but resolution worsens
- ΔE_{mod} reduces with L1 so make L1 large for high resolution (reduces bandwidth)

$$\Delta \mathrm{E}_{\mathrm{mod}} = \frac{2E_i \Delta tmod}{t_i}$$

- For a high resolution instrument like IRIS to maximise flux want $\Delta E_{ana} = \Delta E_{mod}$
- Matching resolution terms just like we did on LET

Optimising an Indirect TOF spectrometer (IRIS)

IRIS resolution

IRIS parameters

Ef=1.84 mev	**Δt_{mod} =120 μs**
L1=36.41 m t_i =61371 μs	**Δd/d=6E-4**
2θ=175°	**Δθ=1.3°**

$$\Delta E_{mod} = \frac{2E_i \Delta tmod}{t_i}$$

ΔE_{mod} = 7.2 μeV

$$\Delta E_{ana} = 2\left(\frac{\Delta d}{d} + cot\theta\Delta\theta\right)\left(\frac{t_f E_i}{t_i} + Ef\right)$$

ΔE_{ana} =3.6 μeV

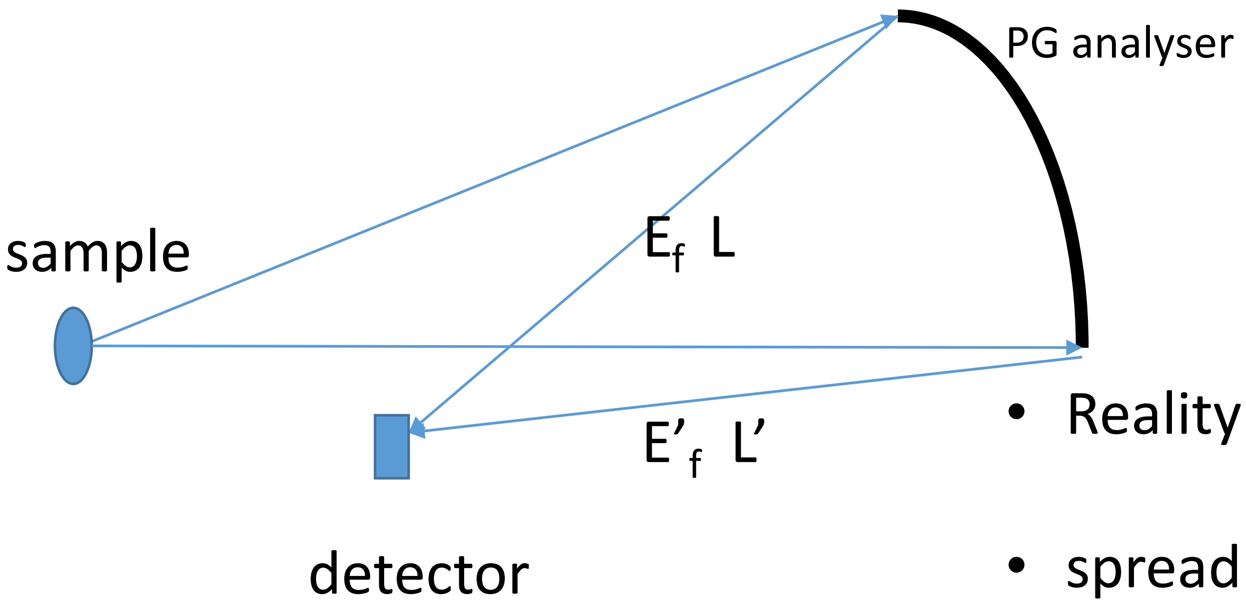
$$\Delta E = \text{sqrt}(\Delta E^2{}_{mod} + \Delta E^2{}_{ana}) = 8\ \mu eV$$

IRIS resolution = 17 μeV   why the large difference?

Optimising an Indirect TOF spectrometer (IRIS)

IRIS resolution

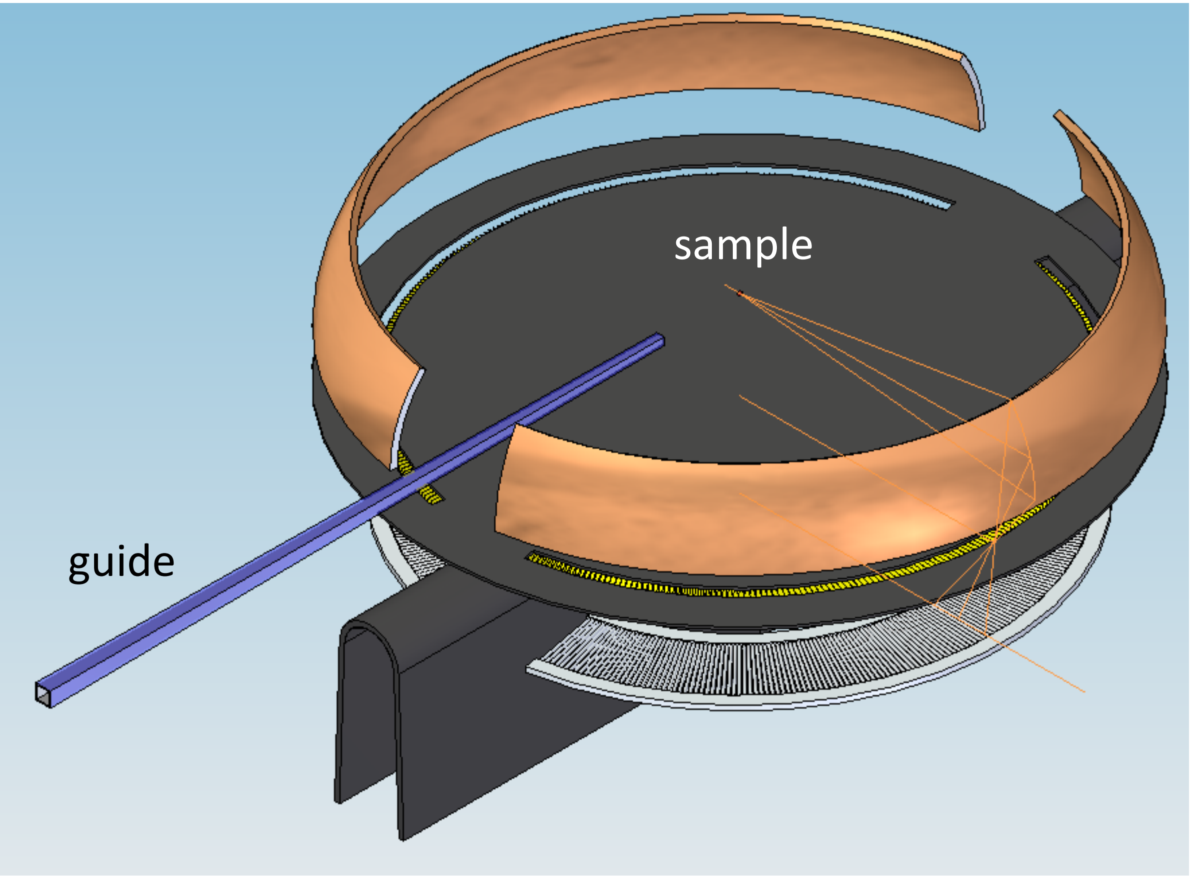
- Real resolution worse than calculated due to analyser size



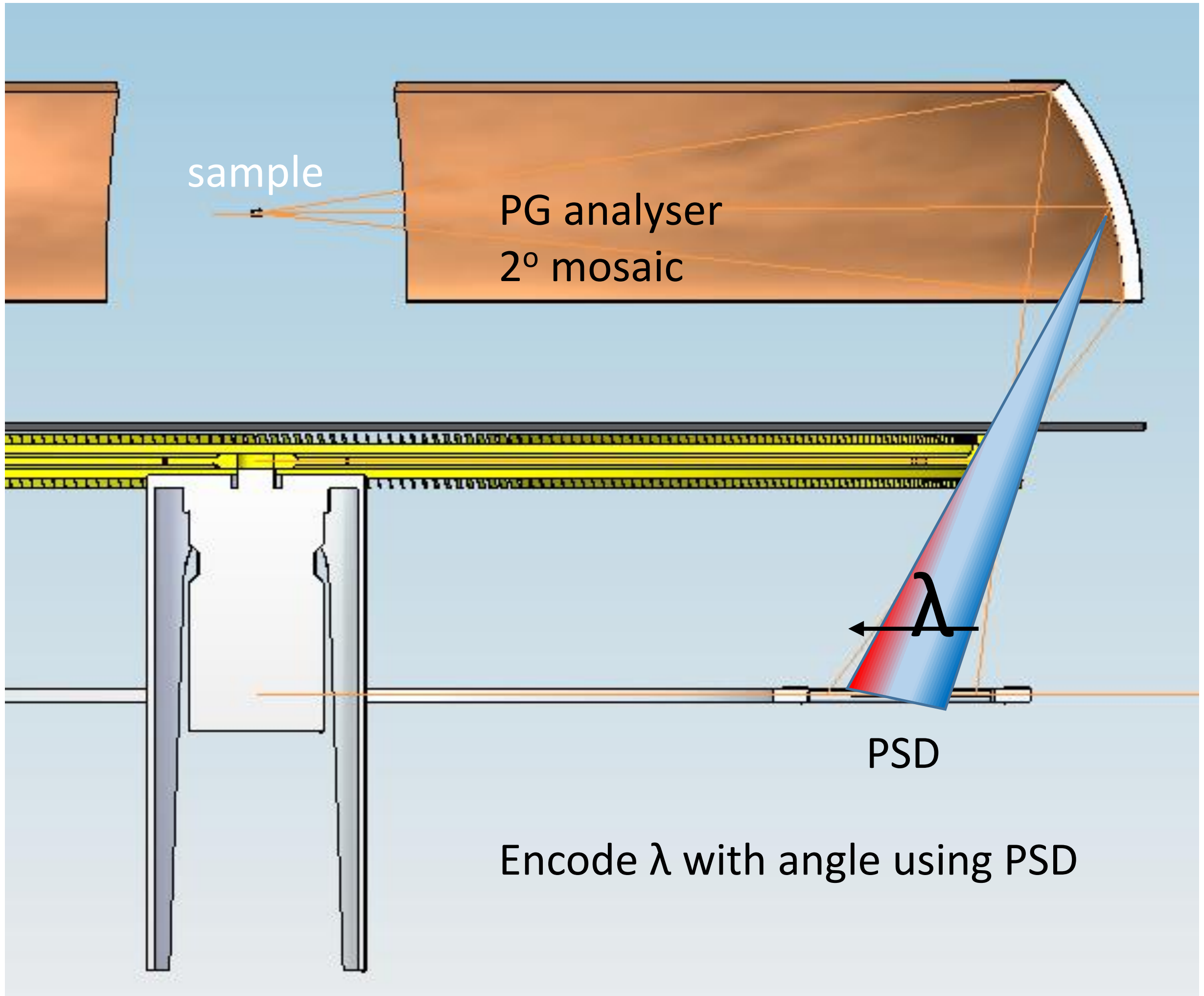
- Reality of a large analyser focussing to a detector
- spread of ΔE_f and ΔL degrade resolution

Nearly all the pain in designing in-direct is how to reduce spread of final energies Ef and path lengths L

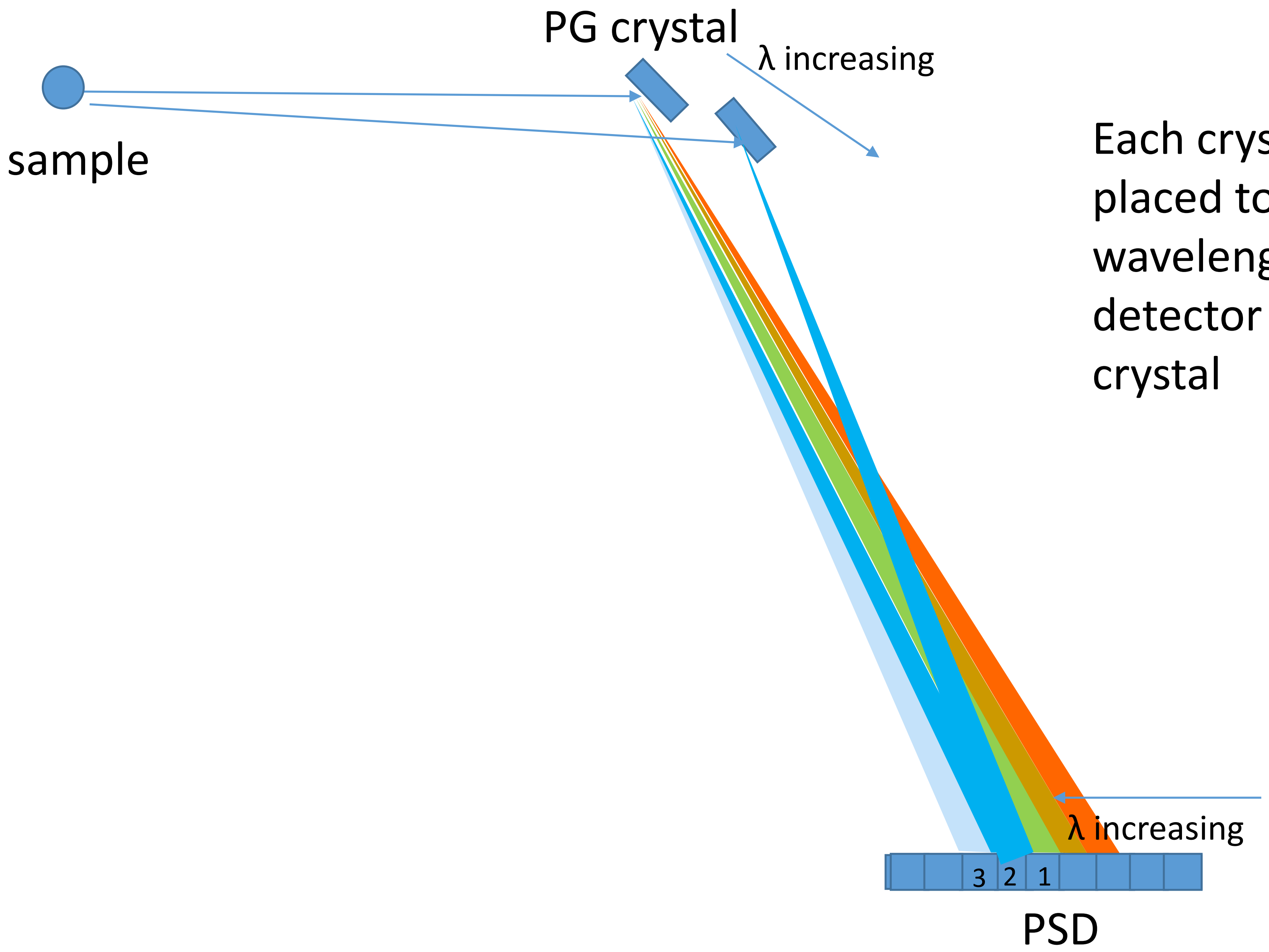
MUSHROOM



Use prismatic effect of PG crystals



MUSHROOM

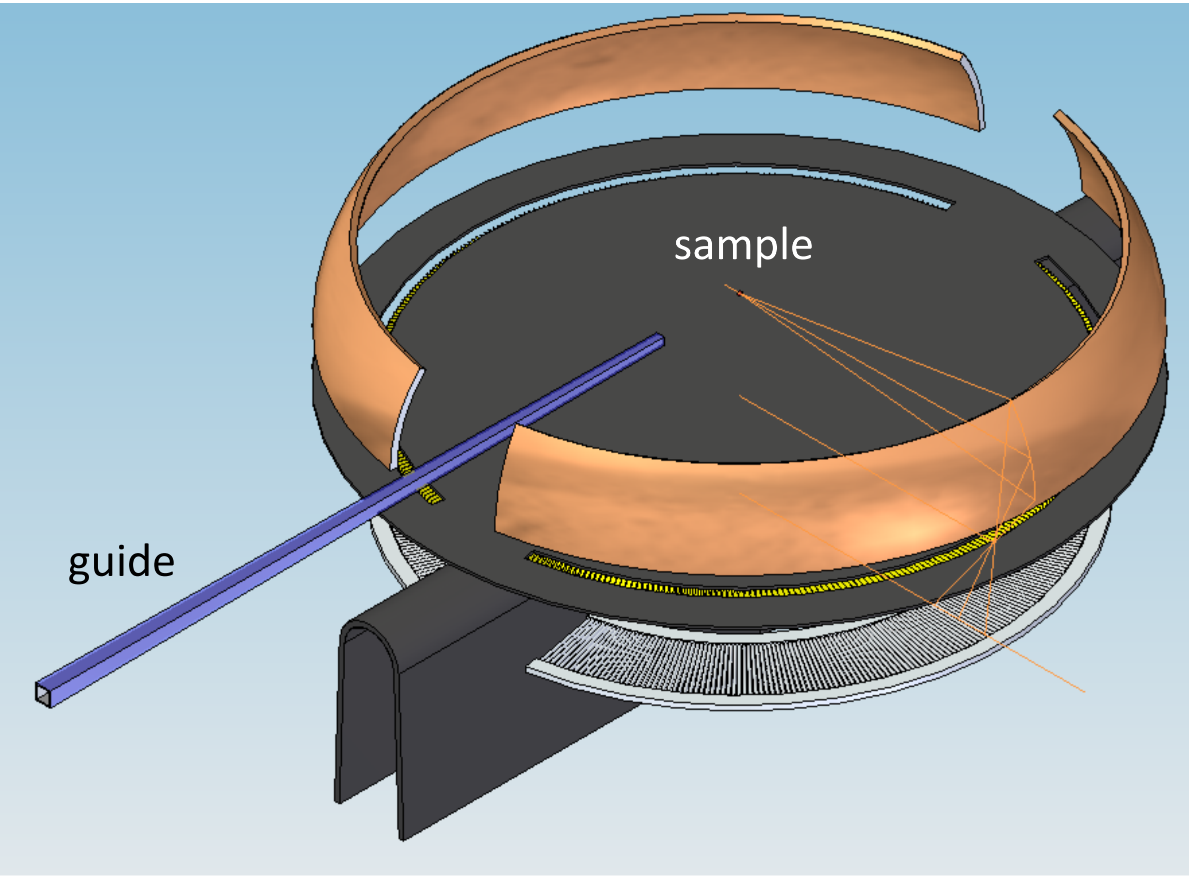


Each crystal in analyser placed to 'mesh' with wavelength spread at detector from previous crystal

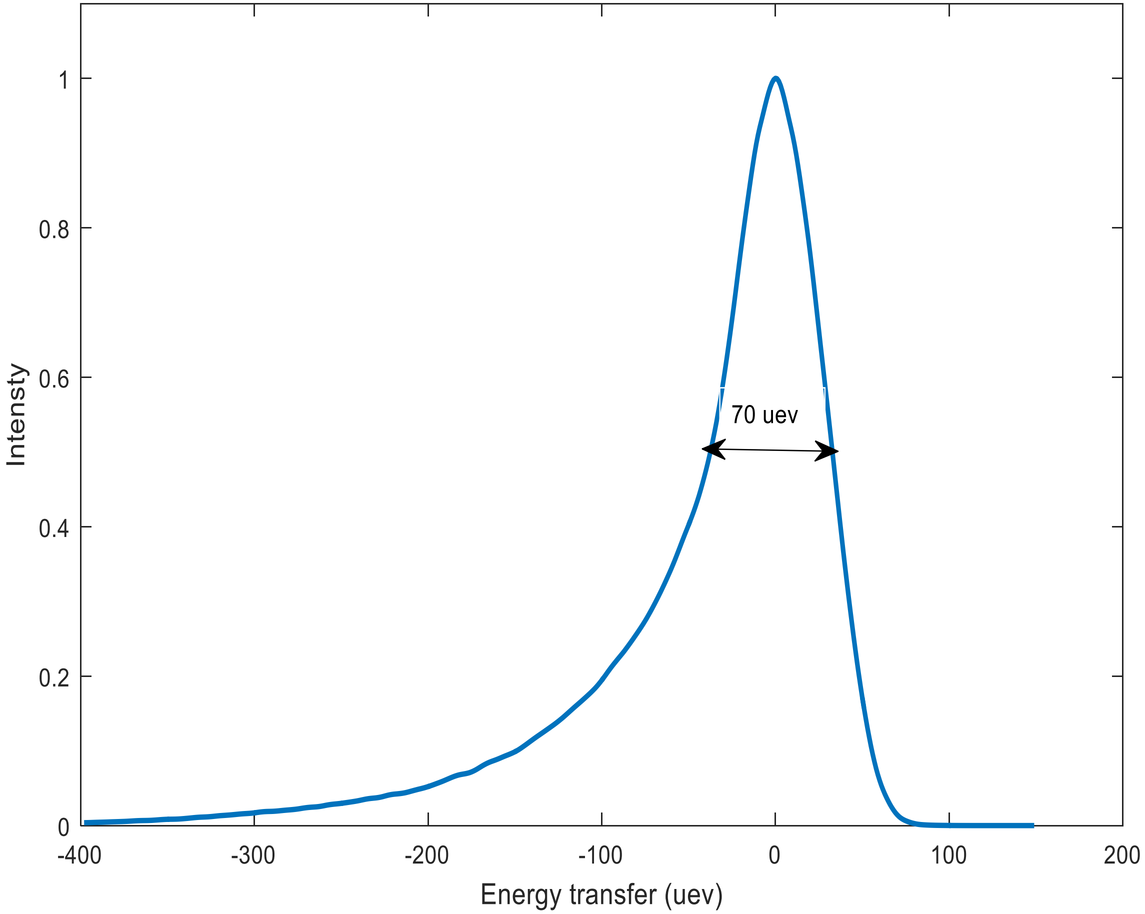
Analyse each detector pixel separately

MUSHROOM

Mushroom has 70 μeV resolution (elastic)
Would be 260 μeV without λ encoding



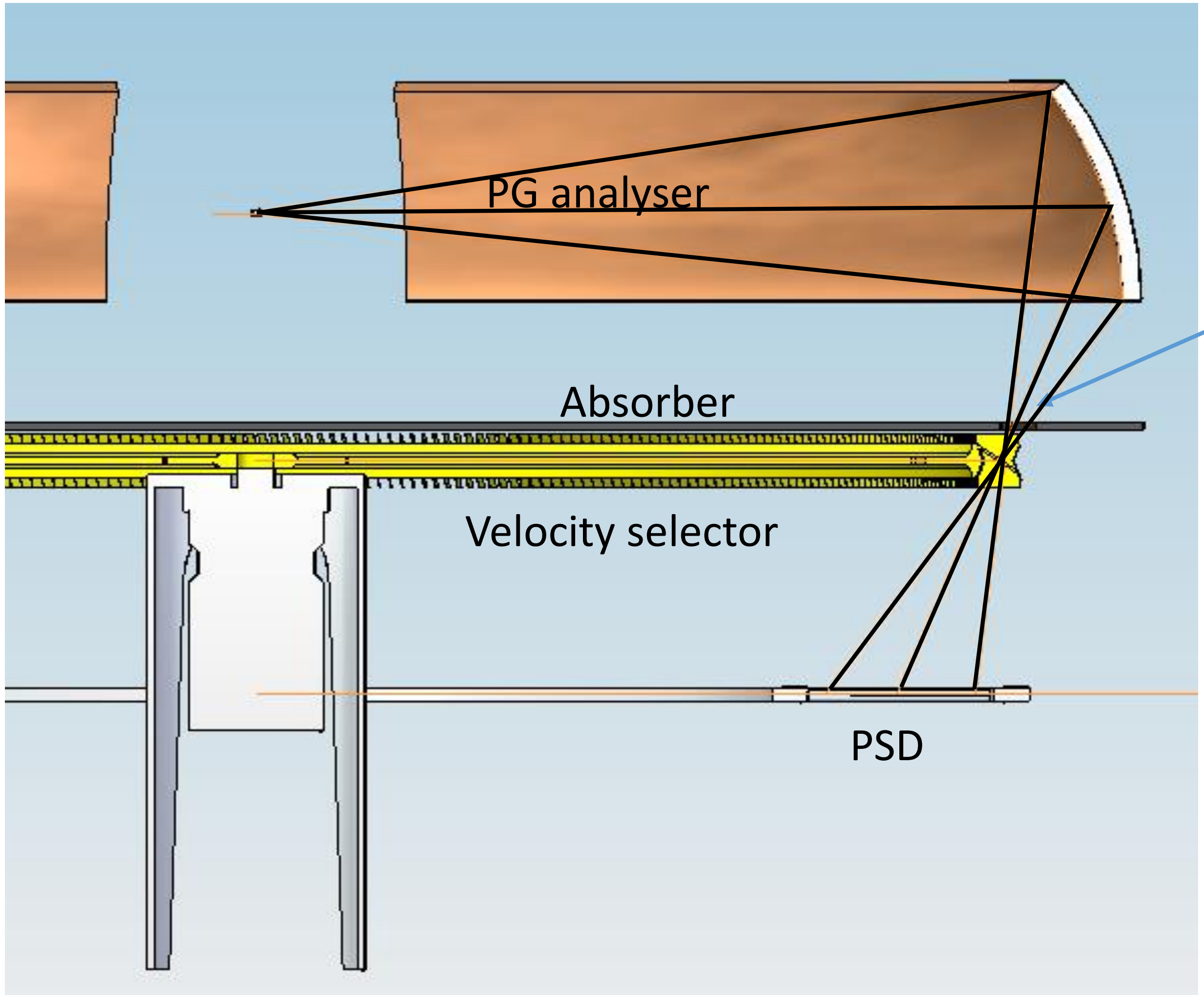
McStas simulations



The large Δλ range accepted by analyser gives 50 x flux of LET at same resolution

MUSHROOM

background minimisation



Neutron all focus though a point at velocity selector

Point on detector can only see point on analyser to minimised background from thermal scattering from PG crystals

Mushroom designed to maximise signal/background

Optimising a TOF spectrometer

SUMMARY

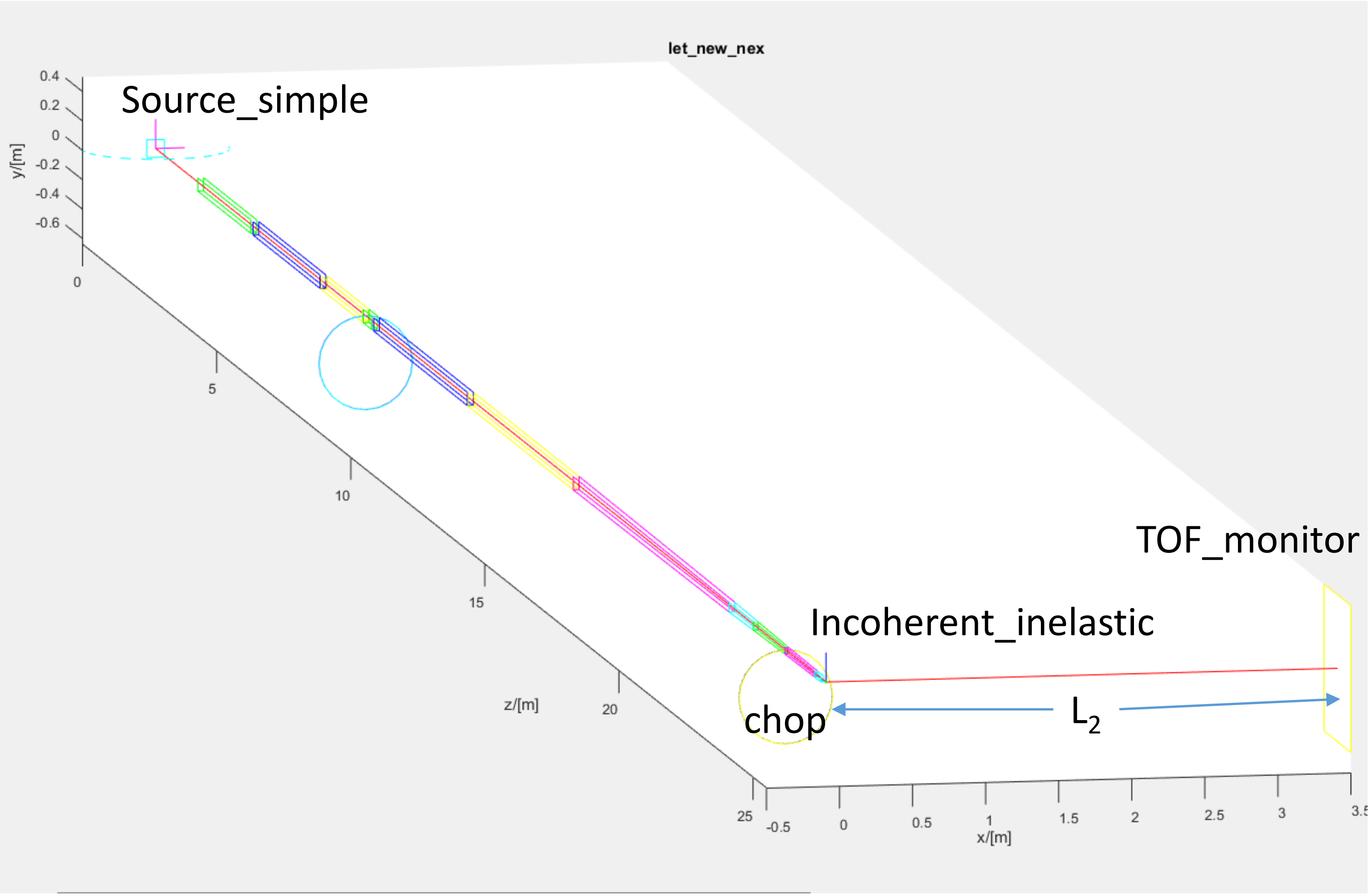
- Don't start with McStas
- Know your key drivers
- FOM is signal/background
- Demonstrated how crucial it is to understand the 'Maths' of the instrument
  - -how it relates to resolution
  - -how it relates to count rate
- Without this information you WILL NOT build an optimal instrument

Have not even mentioned guides yet

…………but we will leave that for another day

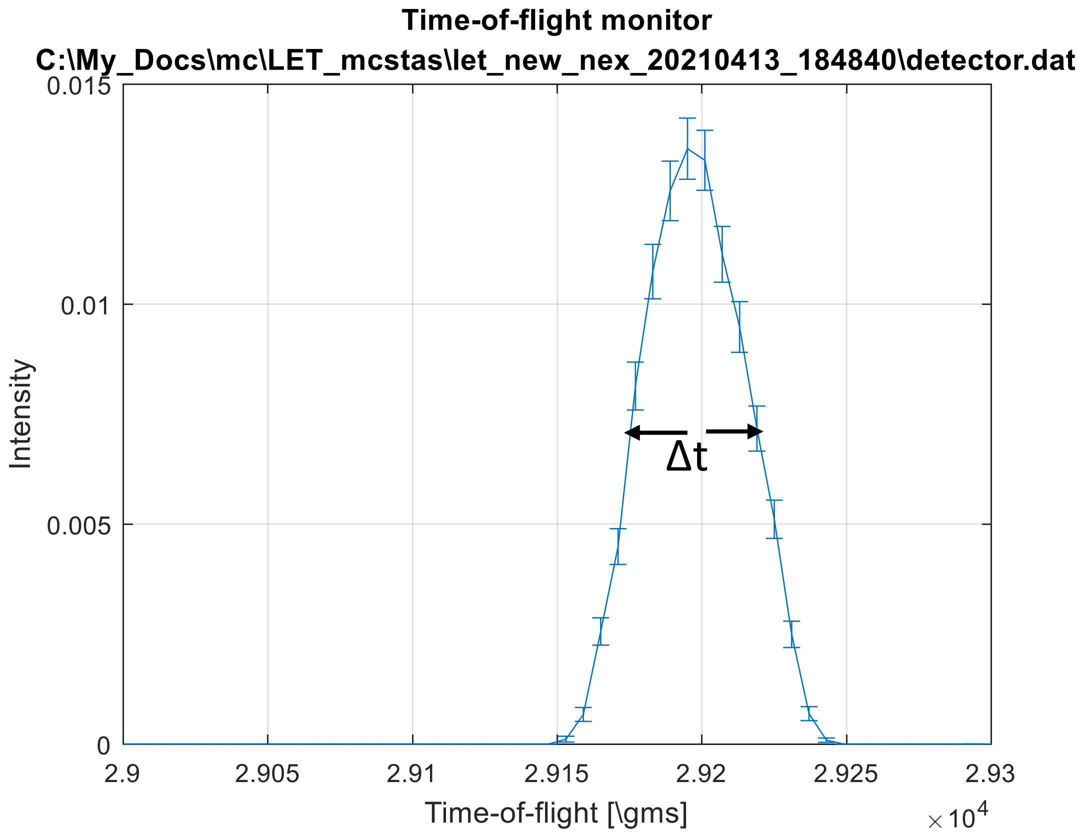
Things to try

Direct geometry



- Keep Ei and chop opening the same
- Scatter to same solid angle
- Vary L_2
- Determine resolution and count rate v L_2

COMPONENT sample=Incoherent_inelastic(
radius=0.005,yheight=0.01,focus_aw=5,
focus_ah=5,target_z=0.0,target_y=0.0,
target_x=1.0)
AT (0, 0, 24.999) RELATIVE Origin



remember

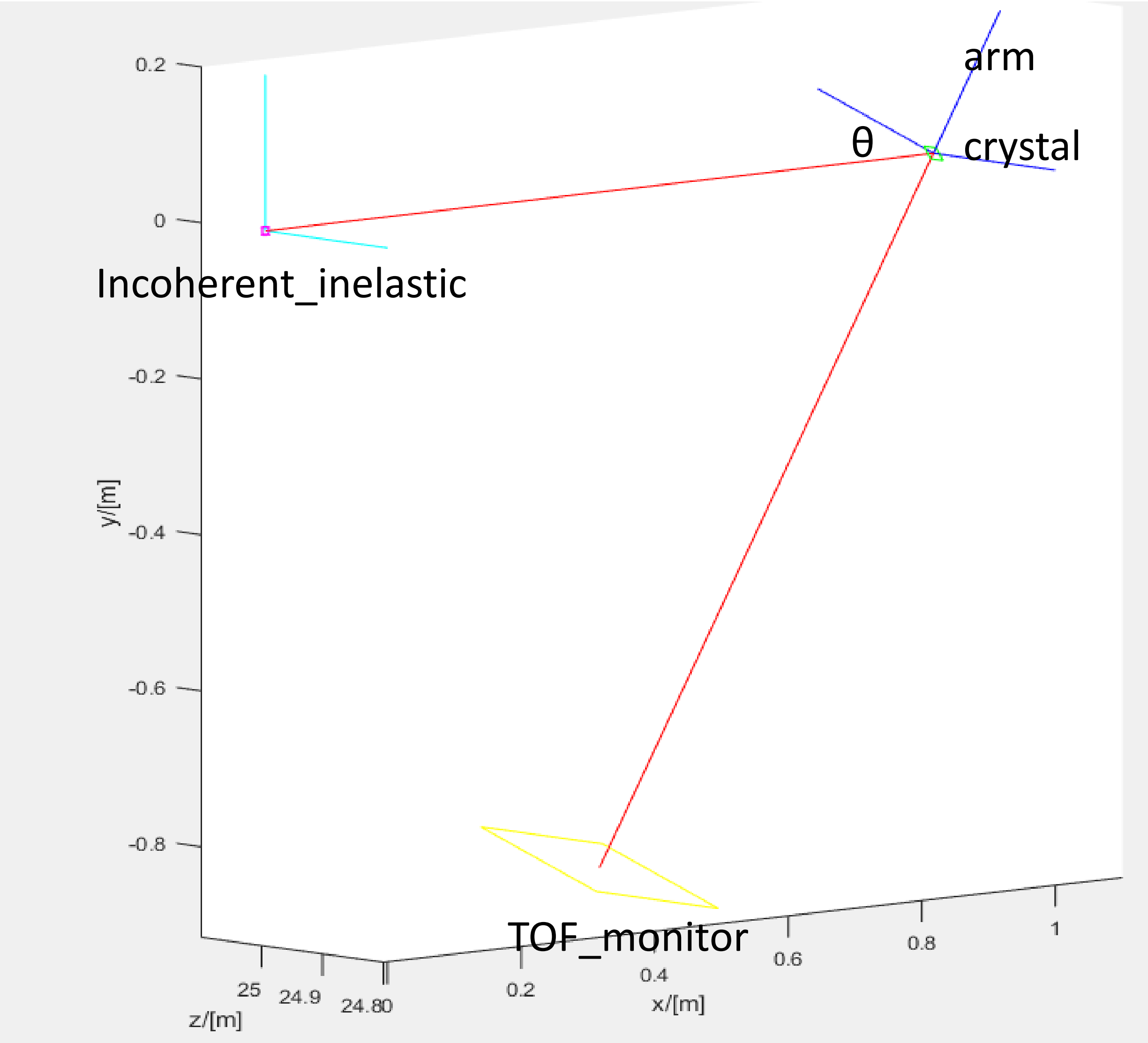
$$\Delta E = \frac{2E_f \Delta t}{t_f}$$

- Elastic so $E_f = E_i$
- know L_2 so calculate t_f
- Get Δt from monitor (it's the FWHM)
- NOW calculate resolution ΔE

- Should be able to predict Δt from geometry and chopper opening
- How does resolution and flux vary with L_2 ………..should be able to predict
- If time. Vary L_2 but keep ΔE constant by varying chopper opening. Plot flux versus L_2

Things to try

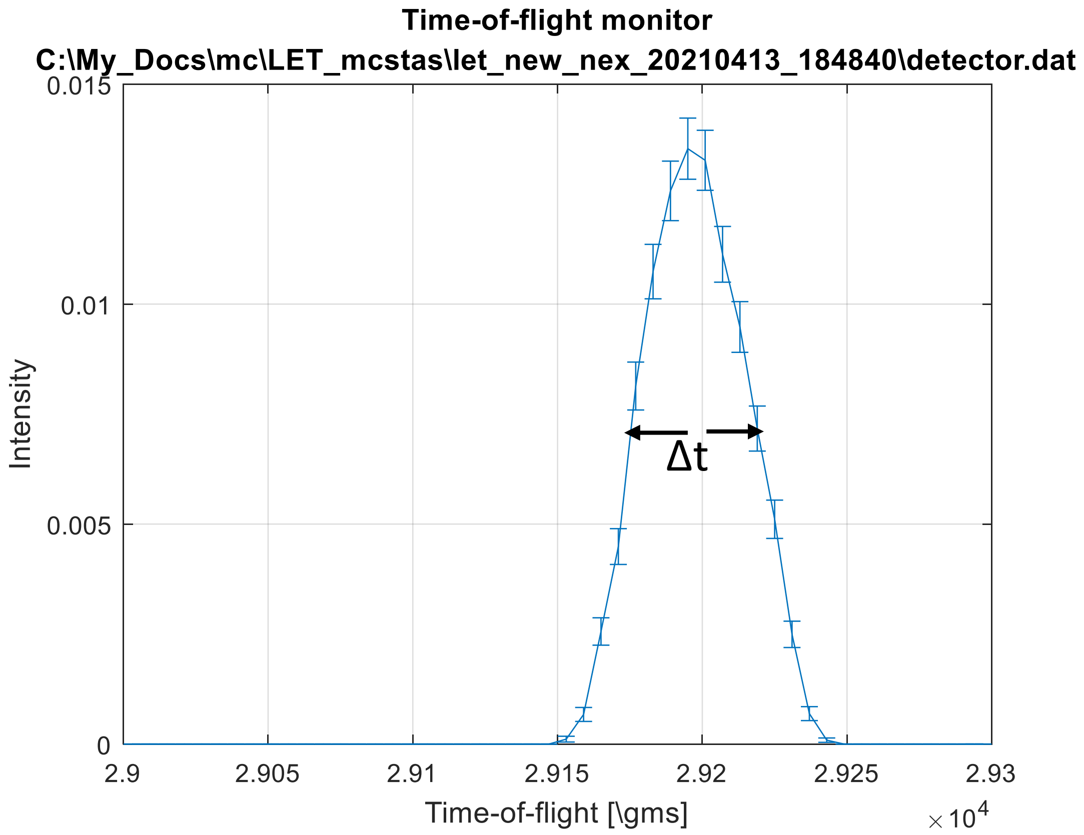
In-direct geometry



- Scatter from incoherent sample to analyser (remember to focus)
- Vary θ
- Determine resolution and count rate v θ

Trick is to use arm component to rotate crystal and TOF_monitor

COMPONENT analyser=Monochromator_flat(zwidth=0.02, yheight=0.02, mosaich=120.0, mosaicv=120.0,Q=1.8734)
AT (0,0,1) RELATIVE detectorarm
ROTATED (-rot, 90,0) RELATIVE detectorarm



remember

$$\Delta E = \frac{2E_i \Delta t}{t_i}$$

- Elastic so $E_f = E_i$
- know L_1 so calculate t_i
- Get Δt from monitor (it's the FWHM)
- NOW calculate resolution ΔE

- Should be able to predict Δt from geometry and crystal angle
- How does resolution and flux vary with θ ………..should be able to predict

My solution Direct

```
DEFINE INSTRUMENT LET_Mantid(E0=5, dE=0.1, Res5=240,slit=0.028,L2=3.5)

DECLARE
%{
double v_foc;
double lam_min,lam_max,den;

%}

// #include <math.h>

INITIALIZE
%{
v_foc = SE2V*sqrt(E0);
%}

TRACE

COMPONENT Origin = Arm()
  AT (0,0,0) ABSOLUTE

COMPONENT Source = Source_simple(radius=0.05, dist=1.7, focus_xw=.04, focus_yh=.09, E0=E0, dE=dE)
  AT (0, 0, 0) RELATIVE Origin

COMPONENT guide1 = Guide_channeled(
    w1 = 0.04, h1 = 0.09, w2 = 0.02, h2 = 0.04868, l = 22.68, alphax = 4.38, alphay = 4.38 ,
 W=3e-3, mx = 4, my = 4)
 AT (0, 0, 1.7) RELATIVE Origin
```

My solution Direct

```
COMPONENT funnel = Guide_channeled(
   w1 = 0.031, h1 = 0.05711, w2 = 0.02, h2 = 0.04868, l = 1.117, alphax = 4.38, alphay = 4.38 ,
 W=3e-3, mx = 4, my = 4)
 AT (0, 0, 22.373) RELATIVE Origin

COMPONENT Res5 = Chopper(
   R = 0.320, f = 2*PI*Res5, n=2, w=slit, pha=23.496/v_foc)
  AT (0, 0, 23.496) RELATIVE Origin

COMPONENT Res5_counter = Chopper(
   R = 0.320, f = -2*PI*Res5, n=2, w=slit, pha=-23.504/v_foc)
  AT (0, 0, 23.504) RELATIVE Origin


COMPONENT endguide = Guide_channeled(
   w1 = 0.02, h1 =0.0484 , w2 = 0.020, h2 = 0.04, l = 1.1, alphax = 4.38, alphay = 4.38 ,
 W=3e-3, mx = 4, my = 4)
 AT (0, 0, 23.52) RELATIVE Origin

COMPONENT snot = Guide_channeled(
   w1 = 0.02, h1 =0.04 , w2 = 0.02, h2 = 0.04, l = 0.23, alphax = 4.38, alphay = 4.38 ,
 W=3e-3, mx = 4, my = 4)
 AT (0, 0, 24.622) RELATIVE Origin

COMPONENT sample = Incoherent_inelastic(radius=0.005,yheight=0.01,efmin=2.5,efmax=6.5,
     focus_aw=5, focus_ah=5,target_z=0.0,target_y=0.0,target_x=1,sigma_abs=0, sigma_inc=5.08)
 AT (0, 0, 24.999) RELATIVE Origin

COMPONENT detectorarm = Arm()
  AT (0, 0,0 ) RELATIVE sample
  ROTATED (0,90.0,0) RELATIVE sample

COMPONENT TOF_target = TOF_monitor(
   nt = 100, filename = "detector.dat",xmin = -0.5,
   xmax = 0.5, ymin = -0.5, ymax = 0.5, tmin=(1e6*(25+L2)/v_foc)-200, tmax =(1e6*(25+L2)/v_foc)+200)
  AT (0, 0, L2) RELATIVE detectorarm
```

My solution to in-direct

```
DEFINE INSTRUMENT LET_Mantid(l0=4,dl=3,rot=0)

TRACE

COMPONENT Origin = Arm()
  AT (0,0,0) ABSOLUTE

COMPONENT Source = Source_simple(radius=0.1, dist=25, focus_xw=.01, focus_yh=.01, lambda0=l0, dlambda=dl)
  AT (0, 0, 0) RELATIVE Origin

COMPONENT sampleMantid = Incoherent_inelastic(radius=0.005,yheight=0.01,efmin=2.5,efmax=6.5,focus_aw=1,
focus_ah=1,target_z=0.0,target_y=0.0,target_x=1,sigma_abs=0, sigma_inc=5.08)
 AT (0, 0, 24.999) RELATIVE Origin

COMPONENT detectorarm = Arm()
  AT (0, 0,0 ) RELATIVE sampleMantid
  ROTATED (0,90.0,0) RELATIVE sampleMantid

COMPONENT graphite_analyser31=Monochromator_flat(zwidth=0.02, yheight=0.02, mosaich=120.0,
mosaicv=120.0,Q=1.8734)
AT (0,0,1) RELATIVE detectorarm
ROTATED (-rot, 90,0) RELATIVE detectorarm

COMPONENT crystalarm = Arm()
AT (0, 0,1 ) RELATIVE detectorarm
ROTATED (-2*rot,0,0) RELATIVE detectorarm

COMPONENT TOF_target = TOF_monitor(
    nt = 1000, filename = "detector.dat",xmin = -0.1,
    xmax = 0.1, ymin = -0.1, ymax = 0.1, tmin=25000, tmax =50000)
  AT (0, 0, -1) RELATIVE crystalarm
END
```