Thermal Spectrometers Comparison
Part II

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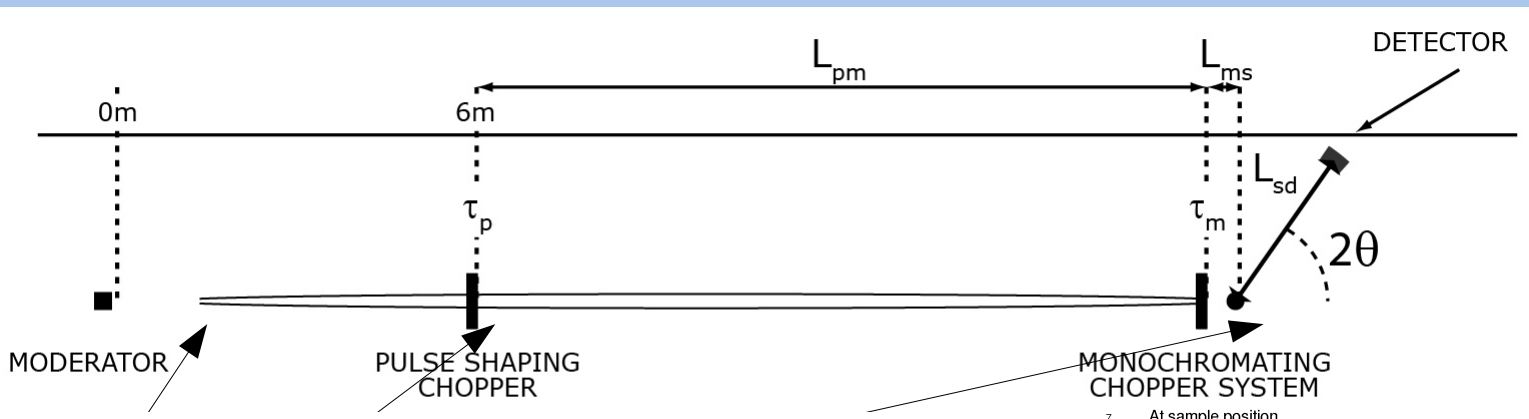
Outline

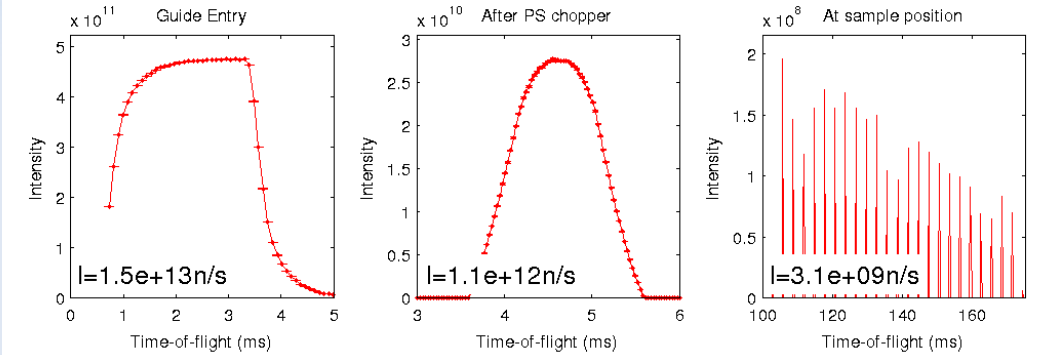
- The McStas 300m Thermal Chopper spectrometer
- Computing the Energy and Q-resolution using McStas
  - The McStas component V_sample
  - The McStas components *TOFRes_sample* and *Res_monitor*
- Virtual data from the 300m Thermal Chopper spectrometer
- Virtual data from the ESS-2011 TAS spectrometer

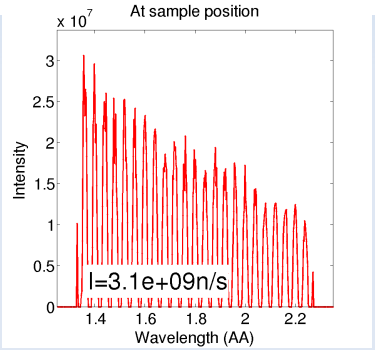
A 300m TOF spectrometer

```
- (Lpm+Lms+Lsd) = 300 m---------------
- Balanced TAUm = 36.6667 mus---------------
- Guide length = 299.58 m---------------
- PS chopper at L2 = 6.58435 m---------------
- mono chopper at L4 = 301.084 m---------------
- MonoChopperSlitA = 9 deg ---------------
- Guide height at MonoChopper = 0.0557082 m ----
- PulseShapingChopperSlitA = 50.4 deg ----------
- omegares = 2*PI* 70 rad/s --------------------
- Actual TAUp = 2 ms ----------------------
- deltaLambda = 0.0199903 Å --------------------
- numOfChopperPulses = 24 ----------------
- omegamono = 2*PI* 336 rad/s ------------------
- Actual TAUm = 37.2024 mus ---------------
- spacing of pulses = 0.0399807 Å --------------
- EI = 25.2467 meV ---------------
```

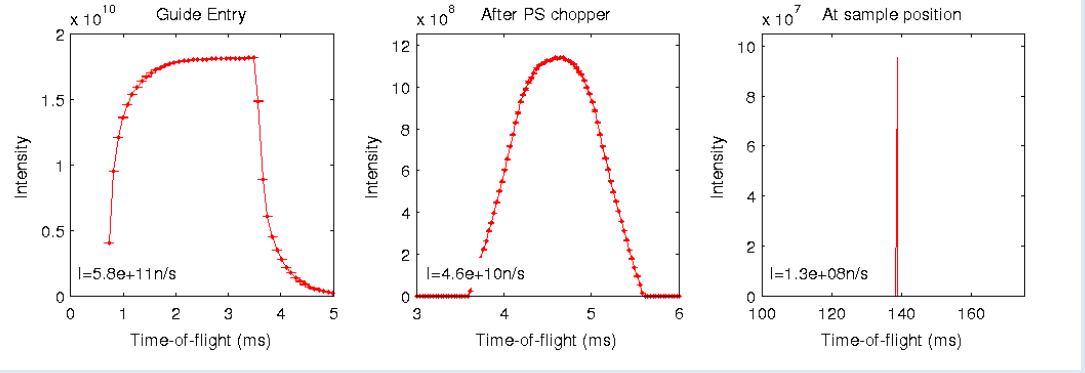


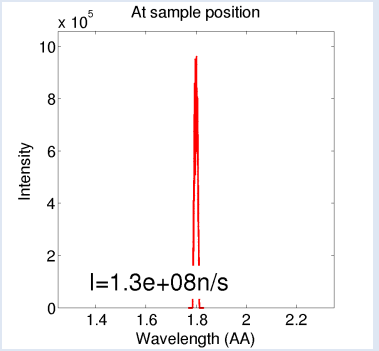
Simulating a 2ms pulse





Simulating a single 37µs pulse





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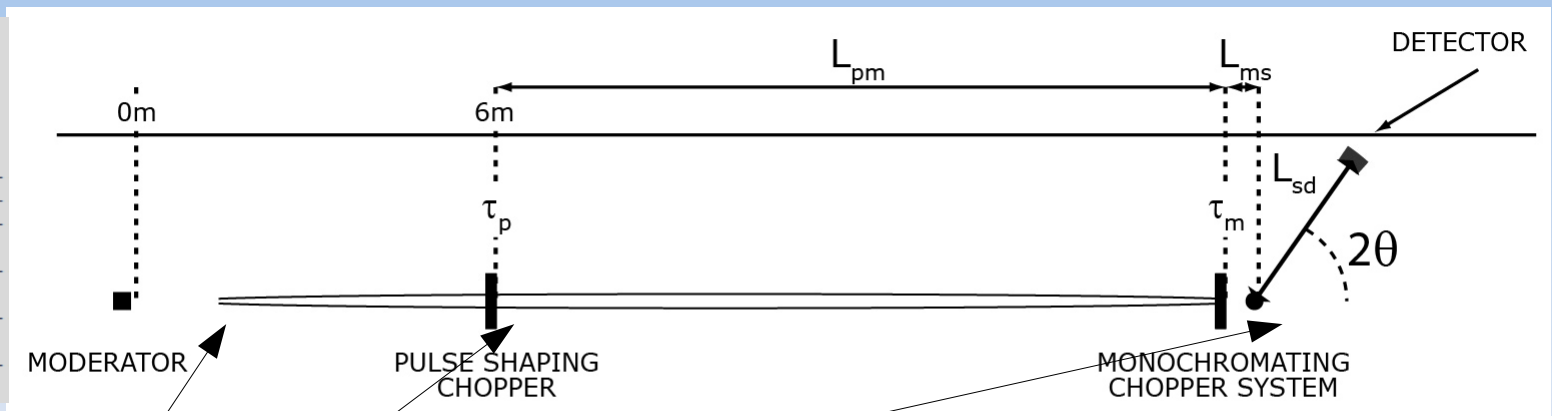

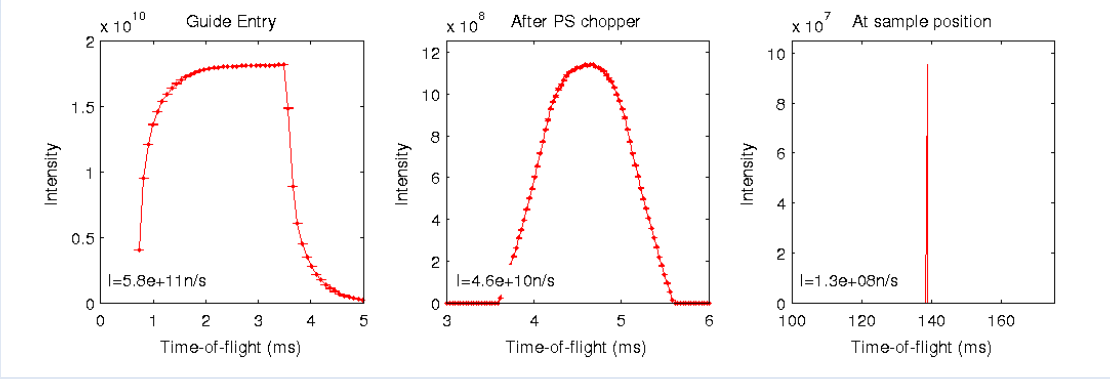

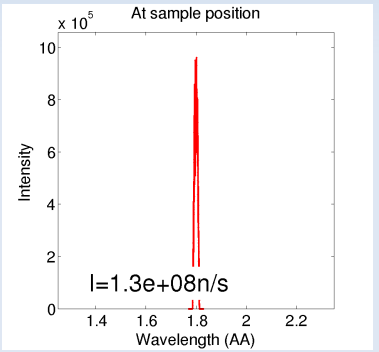

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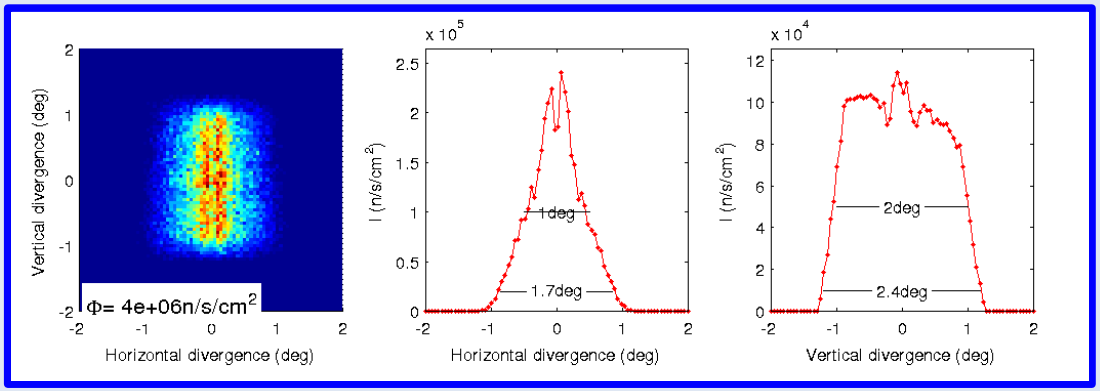
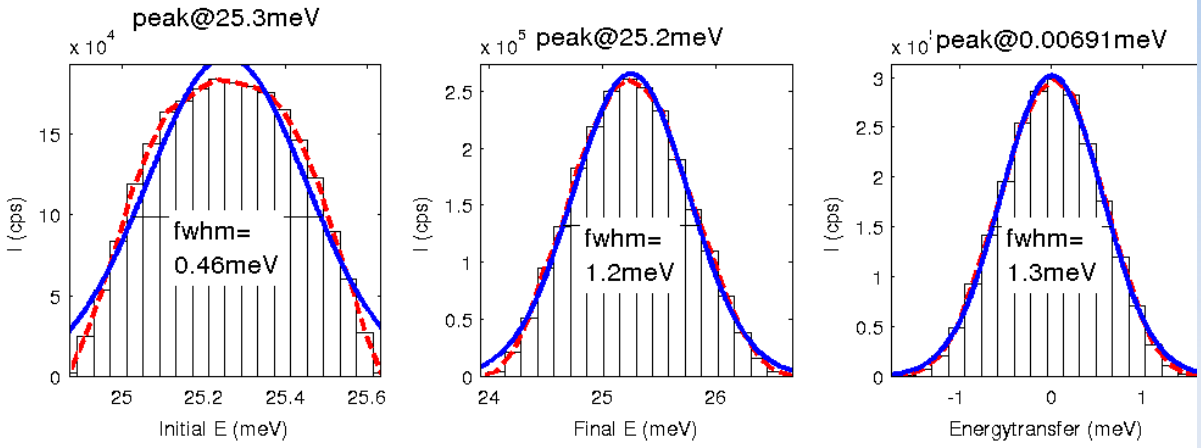
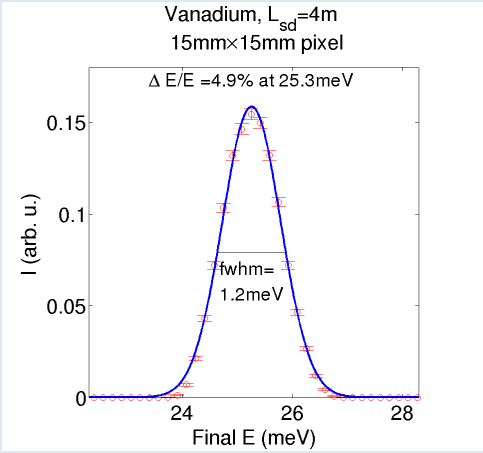


Divergence at sample position

McStas Energy resolution: V_sample and TOFres_sample

E-resolution at TTS=60, zero energytransfer:

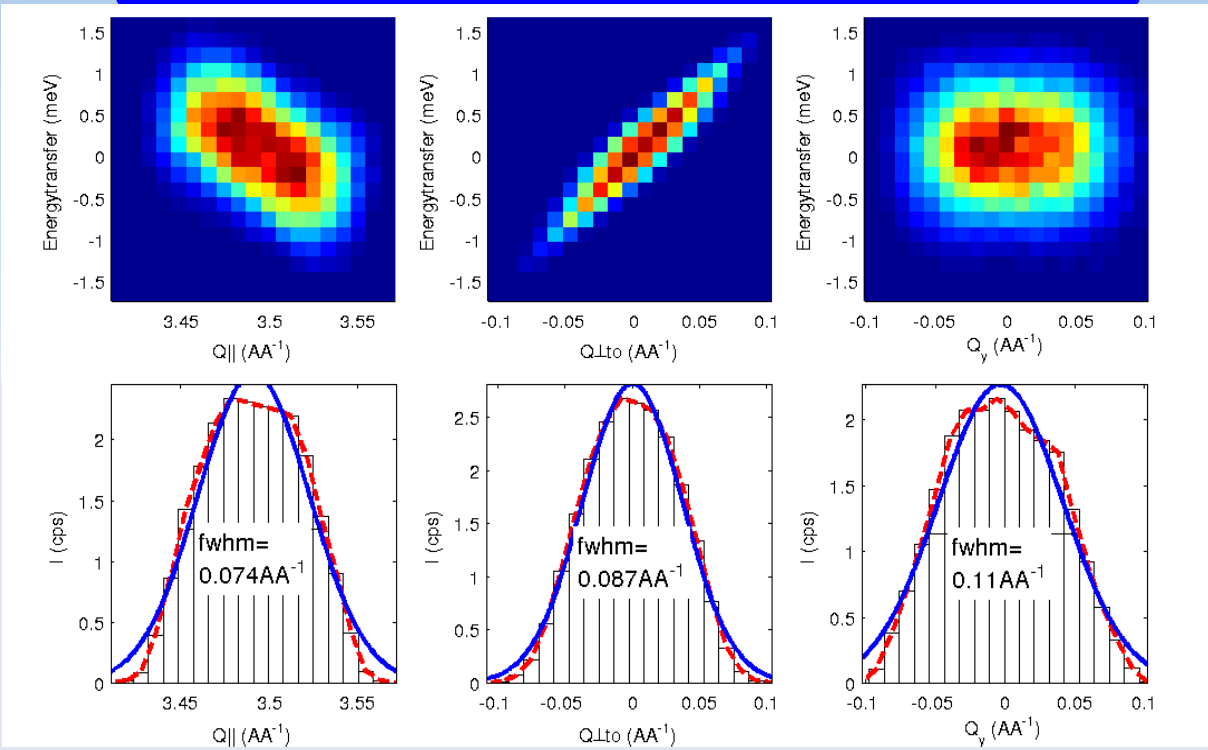




- Elliptic guide (299.6m)
- PS choppers at 6.6m (2ms)
- Mono choppers at 301m (37µs)
- Zoom at single pulse 25.3meV
- Cylindrical sample Ø10mm, h 20mm
- Single detector pixel 15mmX15mm (Lsd=4m)

McStas Q resolution: TOFres_sample

Q-resolution at TTS=60, zero energytransfer:



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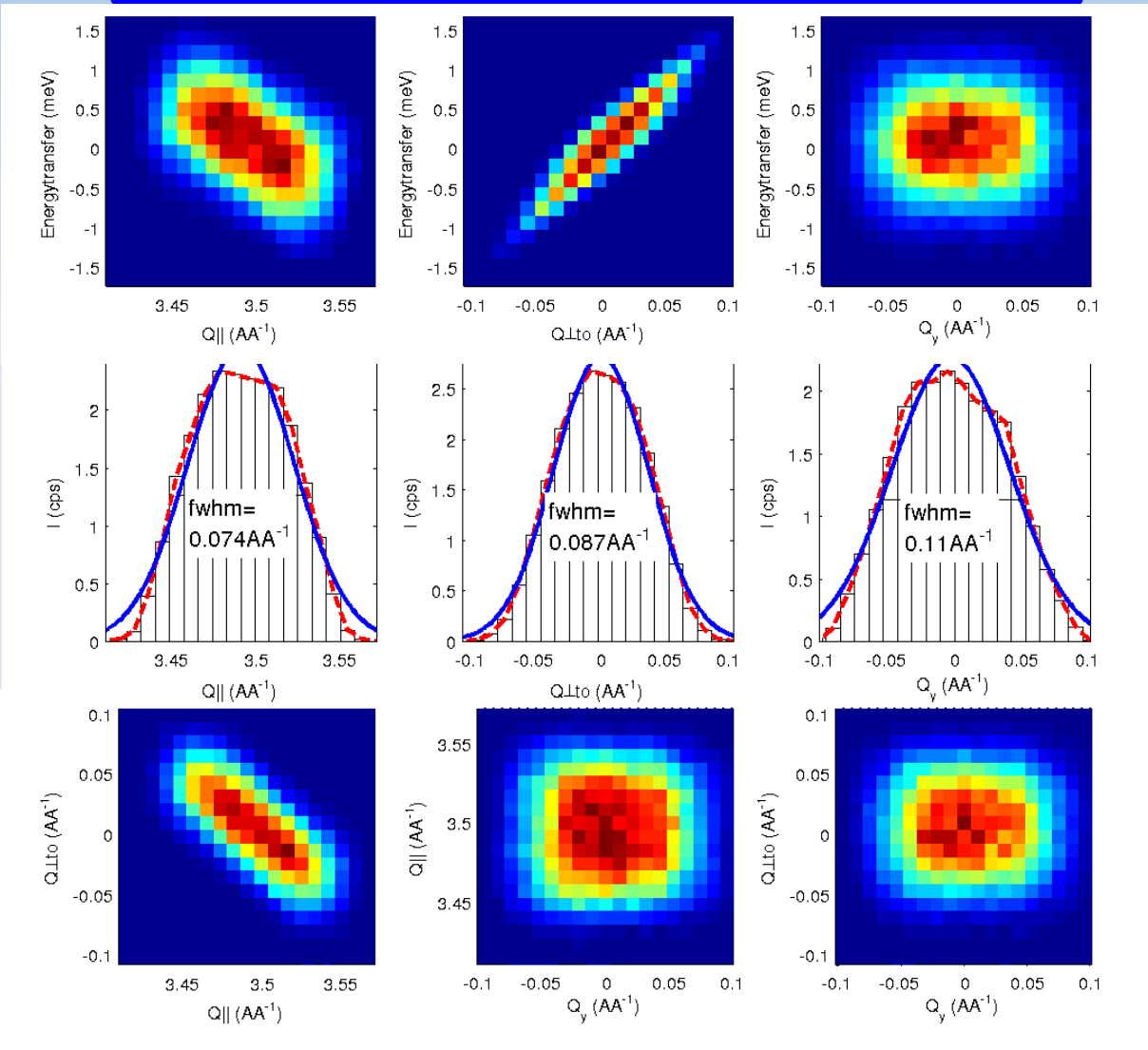

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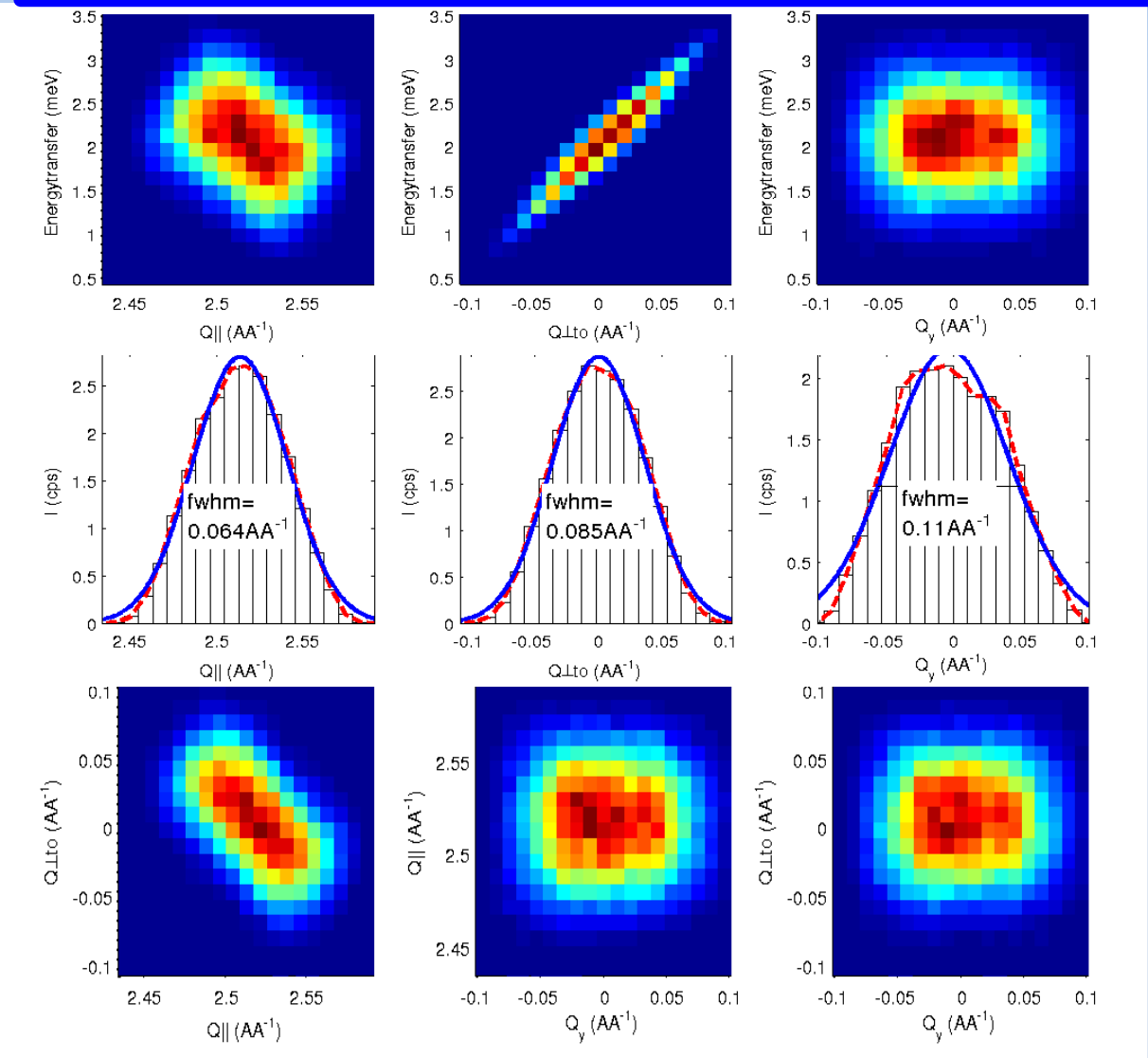
McStas Energy and Q resolution: TOFres_sample

Q-resolution at [002] (Q=2.51Å^{-1}), 2meV energytransfer:



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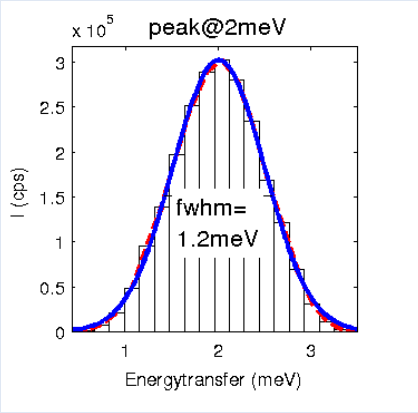
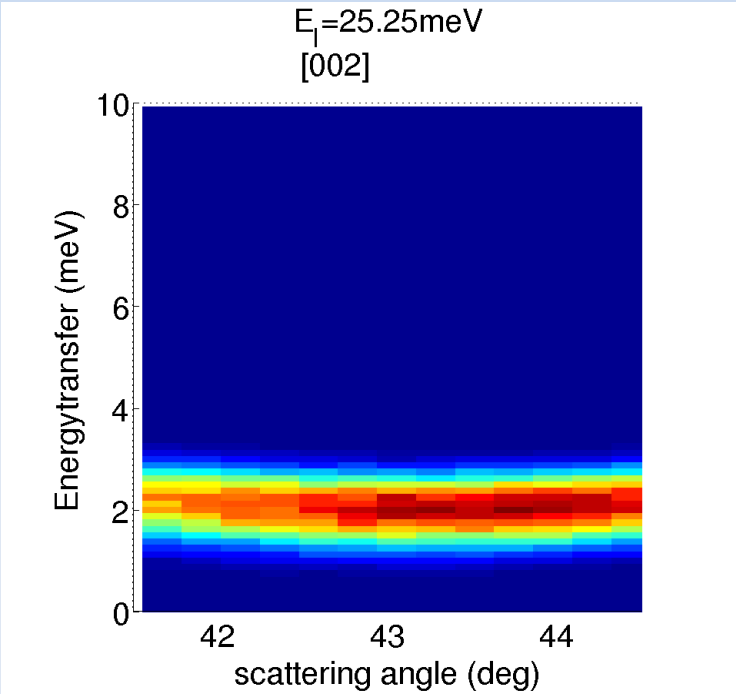
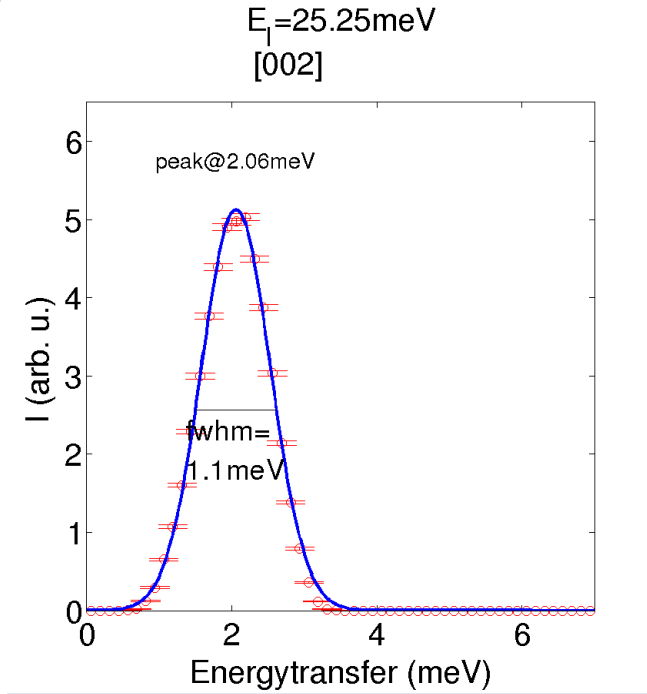
- Zoom at single pulse 25.3meV
- Cylindrical sample Ø10mm, h 20mm
- Single detector pixel 15mmX15mm (Lsd=4m)

E-resolution at [002], 2meV energytransfer:



Virtual experiments: A 300m TOF spectrometer, magnon with a 2meV gap





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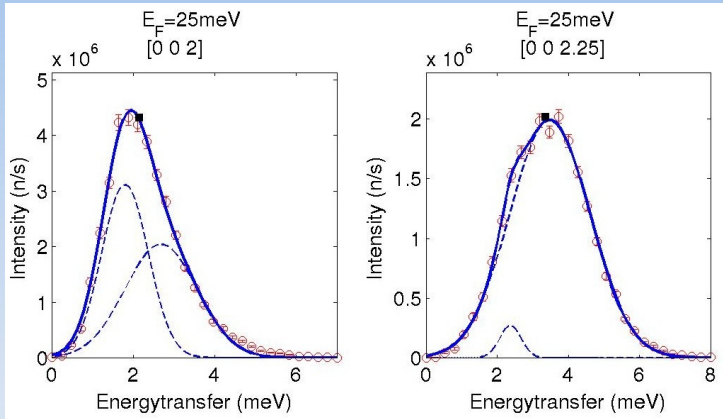
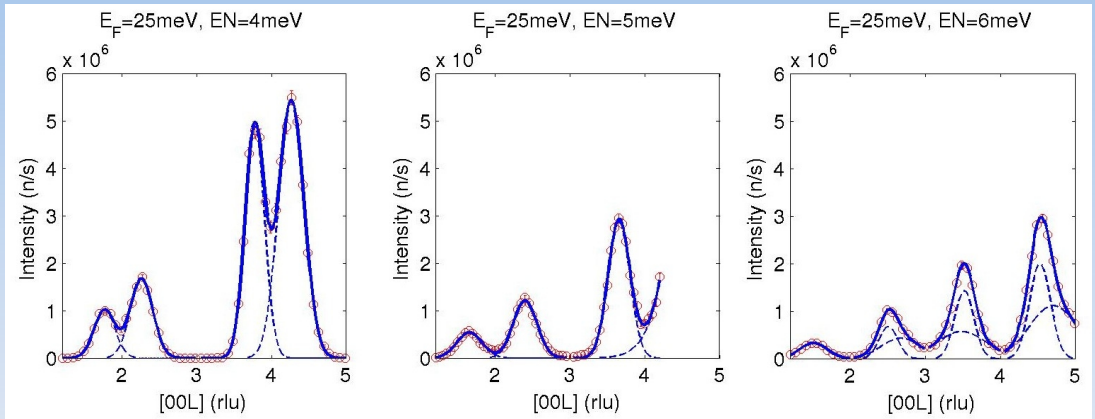
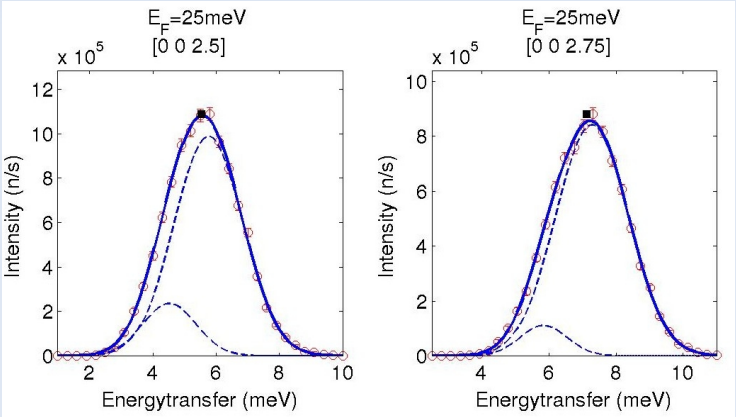
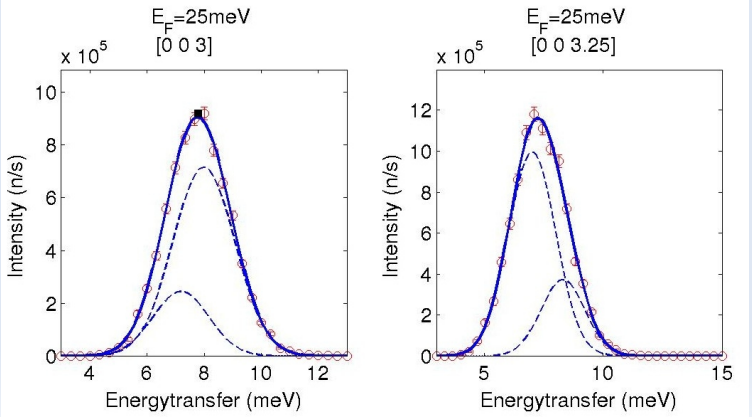
- Zoom at single pulse 25.3meV
- Cylindrical sample Ø10mm, h 20mm
- Single detector pixel 15mmX15mm (Lsd=4m)

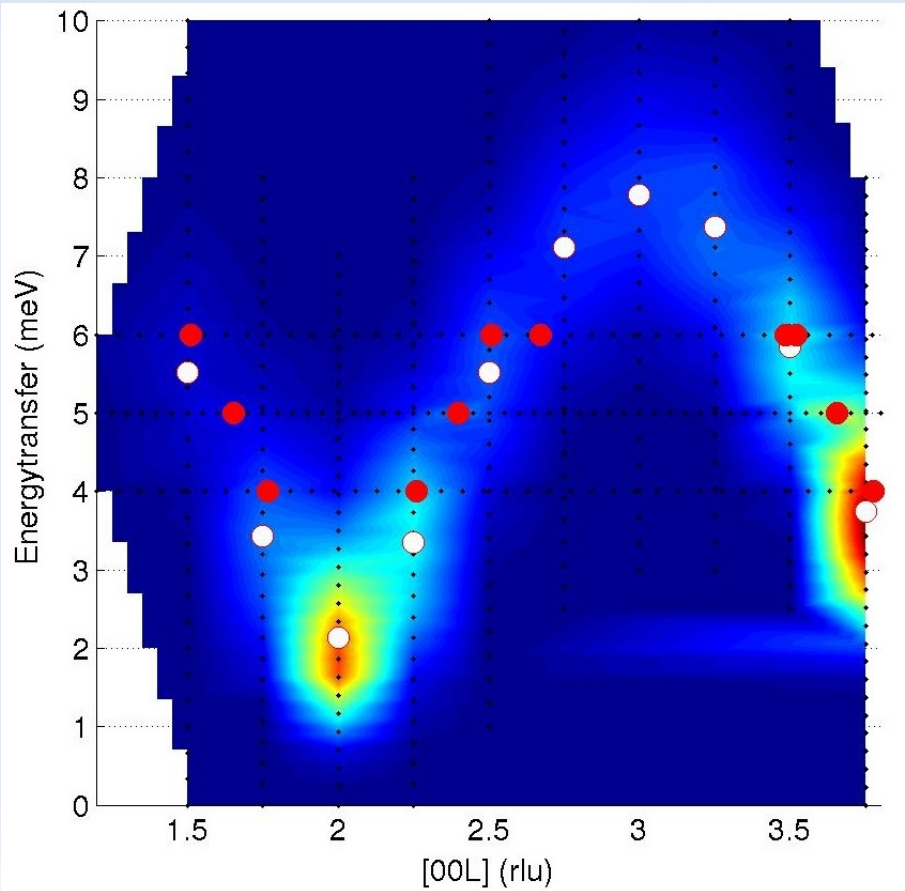
Virtual experiments: ESS-2011 TAS, magnon with a 2meV gap











The McStas components TOFRes_sample and Res_monitor

Physica B 276–278 (2000) 152–153

McStas 1.1: a tool for building neutron Monte Carlo simulations

K. Lefmann[a,*], K. Nielsen[a], A. Tennant[b], B. Lake[c]

The intensity, I, observed in a general neutron experiment may be written as

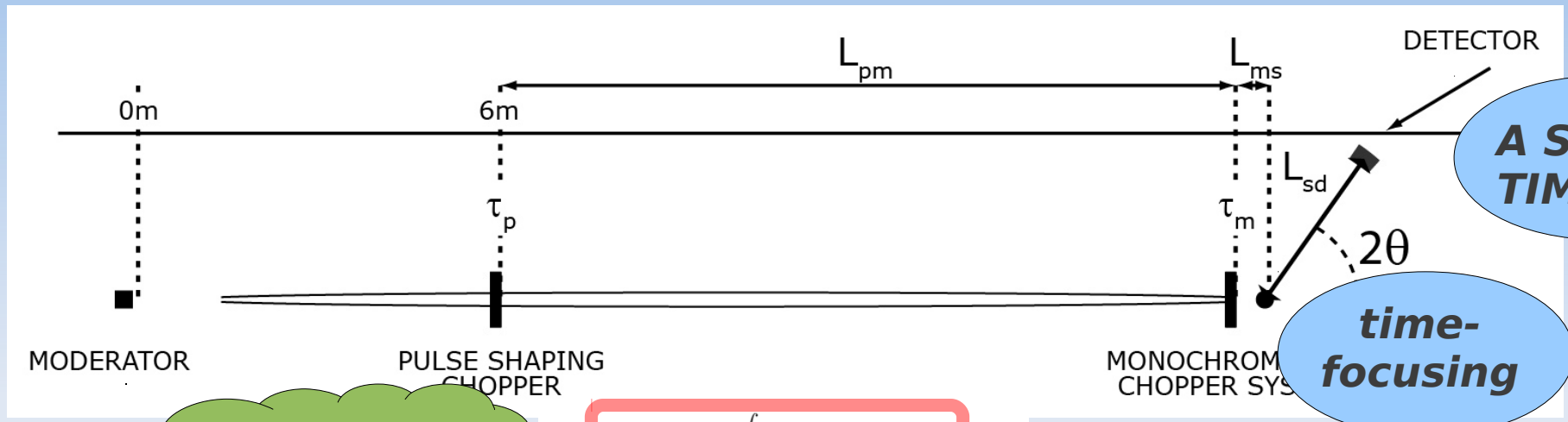
$$I(Q_0, \omega_0) = \int R(Q_0 + \Delta Q, \omega_0 + \Delta\omega)\, \sigma(Q_0 + \Delta Q, \omega_0 + \Delta\omega)\, d(\Delta Q)\, d(\Delta\omega)\,, \qquad (1)$$

where σ is the scattering cross section. R is the resolution function, which is given by

$$R(Q, \omega) = \int_{\text{path}} P(Q, \omega, \text{path})\,, \qquad (2)$$

where $P(Q, \omega, \text{path})$ is the transmission probability for a neutron along the given path and the integral is over all possible paths with the given energy and momentum transfer.

The McStas components TOFRes_sample and Res_monitor



Q, λ, ω
samplesize

$$R(Q,\omega) = \int_{\text{path}} P(Q,\omega,\text{path})\,,$$

List of
kI, kF, (x,y,z)
and
neutron weights p

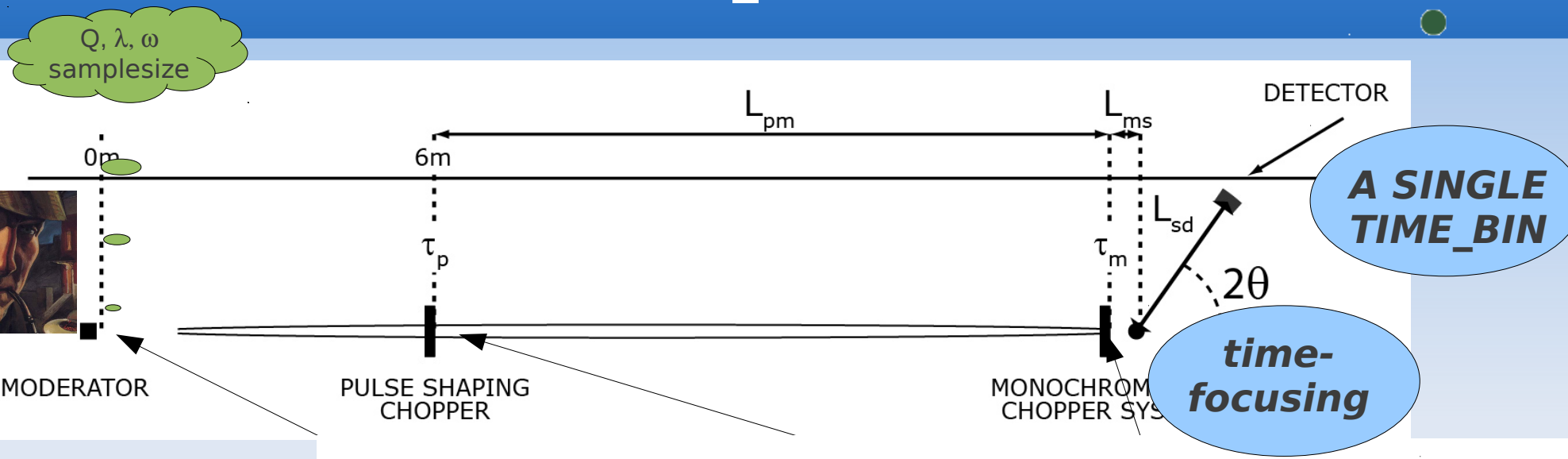
TOFRes_sample.comp

- Written by K. Lefmann in 2004
- Inelastic sample with completely uniform scattering in both solid angle and energy
- ***Time focusing*** is used to optimize the simulations

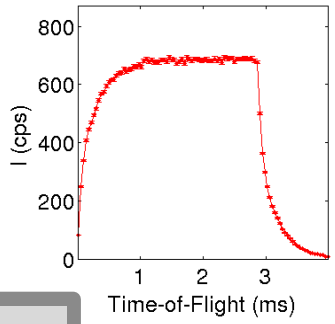
Res_monitor.comp

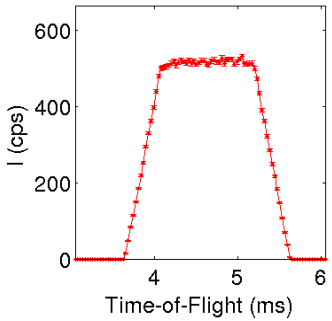
- Written by K. Nielsen in 1999
- Outputs a list of neutron scattering events in the sample along with their intensities at the detector

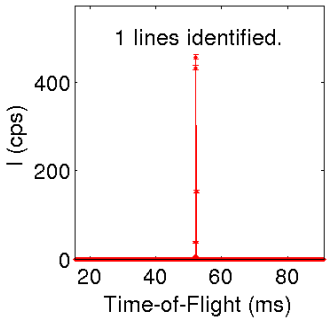
The McStas components TOFRes_sample and Res_monitor

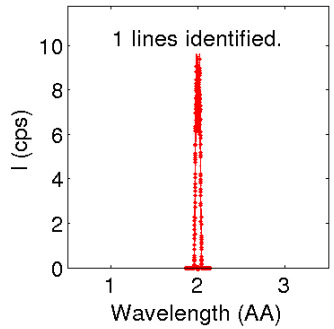



```
-----(Lpm+Lms+Lsd) = 105.5 m----------------
----- Balanced TAUm = 104.265 mus----------
----- MonoChopperSlitA = 16 deg -----------
----- PulseShapingChopperSlitA = 10 deg ---
----- deltaLambda = 0.0941944 Å -----------
----- numOfChopperPulses = 15 -------------
----- omegamono = 1319.47 rad/s -----------
----- TAUm calculated = 105.82 mus --------
----- spacing of pulses = 0.188389 Å ------
```





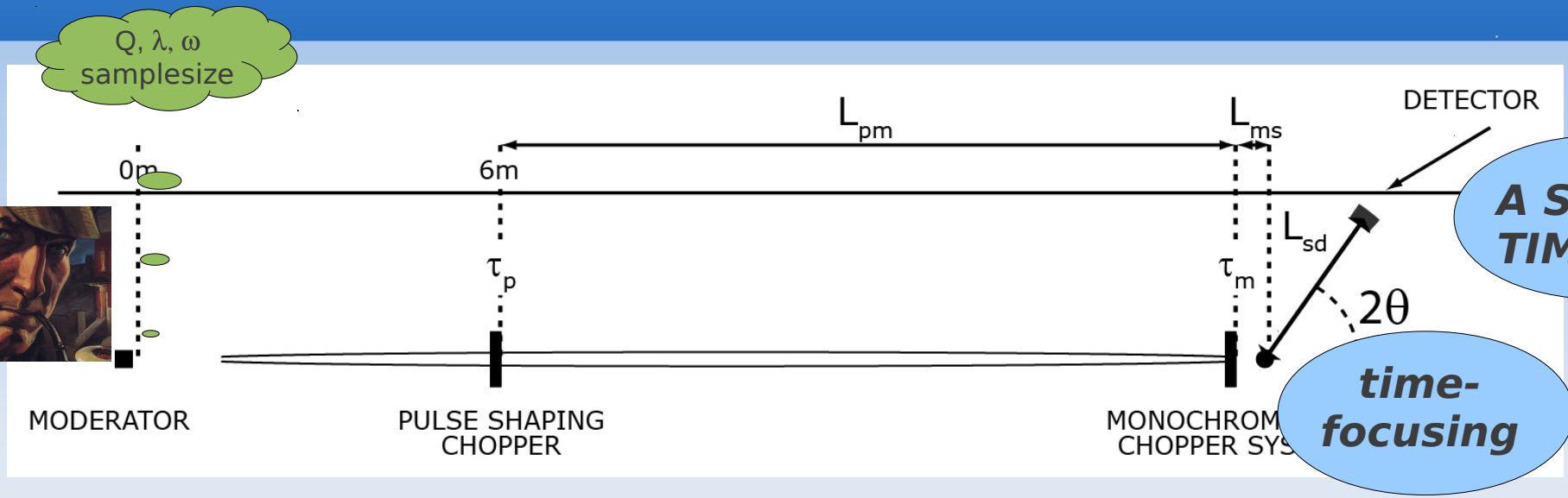





```
-- TTS = 60 deg ---------------
-- Energytransfer is 0 meV for lambda0= 2 Å ---
-- corresponding to  ---------------
-- TIME_BIN = 54934.5 mus----------------
```

```
-- TTS = 60 deg ---------------
-- Energytransfer is 2 meV for lambda0= 2 Å ---
-- corresponding to  ---------------
-- TIME_BIN = 55041.3 mus----------------
```

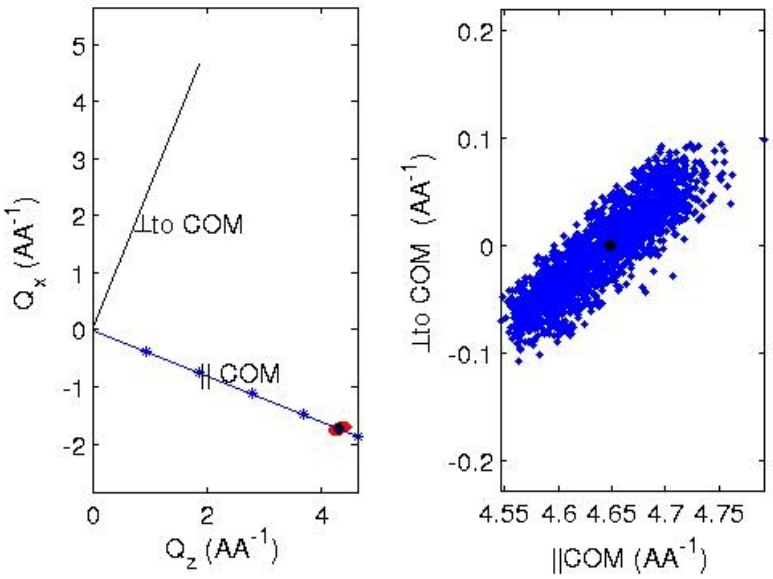
Using McStas to compute the resolution function

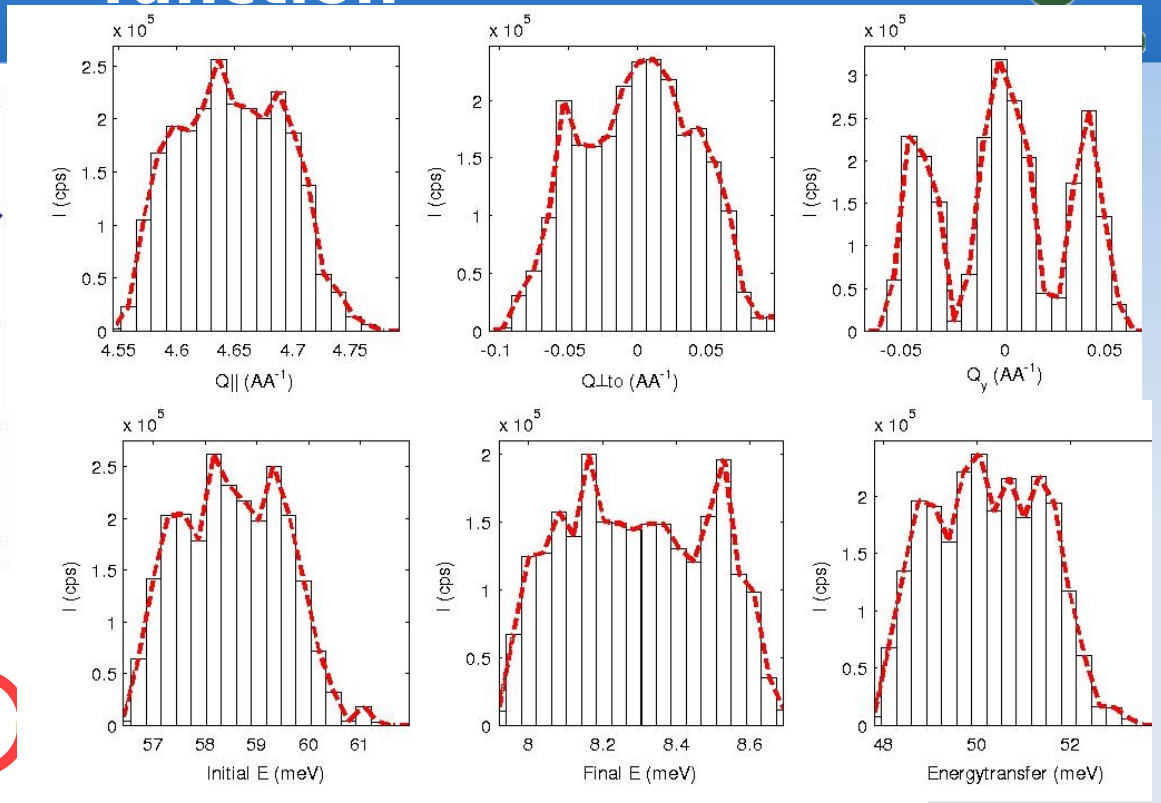


Output file from Res_monitor.comp

```
# xlabel: List of neutron events
# ylabel: ki_x ki_y ki_z kf_x kf_y kf_z x y z p_i p_f
# zvar: I
# zlabel:  Signal
# xylimits: 0 3.40282e+38 1 11 -0.063218 7824.05
# variables: I I_err N
0.00610831 -0.0458673 5.36513 1.70993 -0.00365502 0.985194 -0.00530911 0.00697319 0.00375784 5310.82 1
0.0118866 0.00847943 5.24487 1.75994 0.0058607 1.01107 -0.00163185 -0.0102572 0.00788688 1097.32 1
0.0273682 -0.0419707 5.23393 1.76244 0.00708161 1.01391 0.00120944 -0.0142911 0.00646848 634.402 1
0.00205754 0.0550062 5.31825 1.72412 0.00331141 0.996913 0.000103945 -0.00827845 -0.000349658 0.380685 1
0.0139785 0.0465125 5.25549 1.75107 -0.00259499 1.00878 0.00042111 0.00878956 0.00200478 190.84 1
0.0223152 -0.0583987 5.3031 1.73268 -0.00123379 0.999505 -0.00384755 -0.00121168 6.80198e-05 0.00121296 1
0.00319202 0.0142787 5.30837 1.72783 -0.0076737 0.997157 0.000338551 0.0154559 0.00275913 584.981 1
0.00208033 0.046247 5.299 1.73193 -0.00245527 0.996125 -0.00694022 0.00742765 0.00391925 219.462 1
-0.00757335 -0.0431543 5.3212 1.72598 0.00199661 0.996216 -0.00966691 -0.00101881 -0.000874611 104.542 1
0.0146657 -0.0124116 5.27331 1.73702 0.00432037 1.00778 0.00073683 -0.00831697 -0.00947651 414.621 1
-0.00723267 0.0413729 5.234 1.76285 -0.000101842 1.0144 0.00314663 -0.000772517 0.00655112 170.145 1
```

Using McStas to compute the resolution function



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# ylabel: ki_x ki_y ki_z kf_x kf_y kf_z x y z p_i
# zvar: I
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# xylimits: 0 3.40282e+38 1 11 -0.063218 7824.05
# variables: I I_err N
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0.0118866 0.00847943 5.24487 1.75994 0.0058607 1.01107 -0.00163185 -0.0102572 0.00788688 1097.32 1
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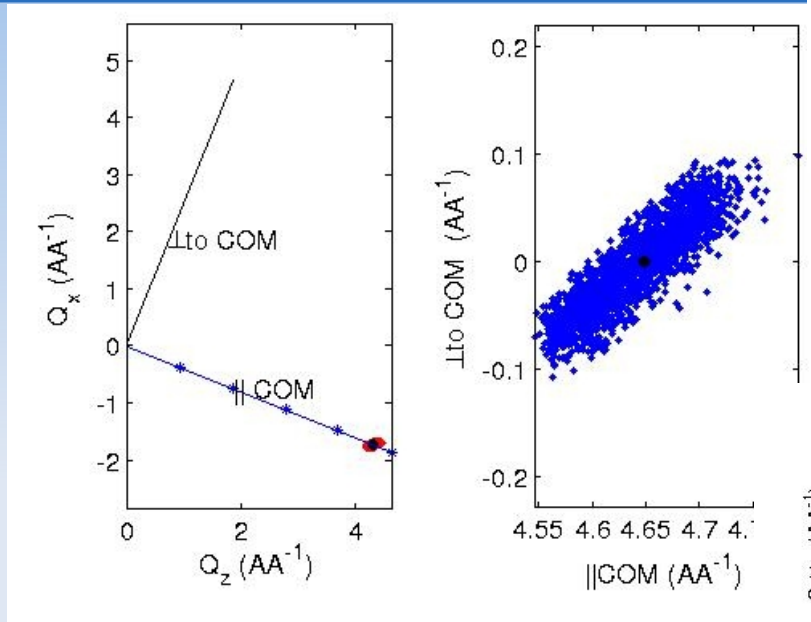

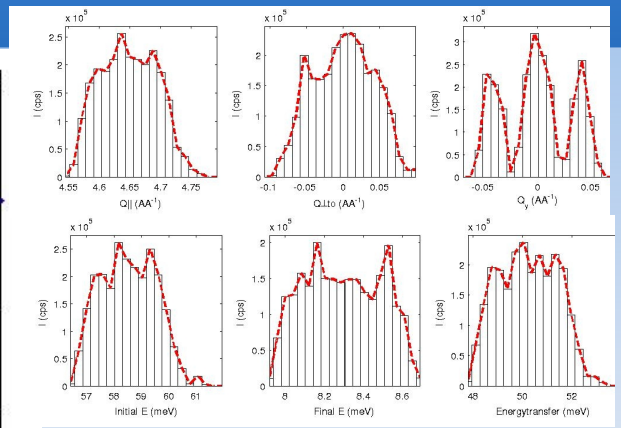

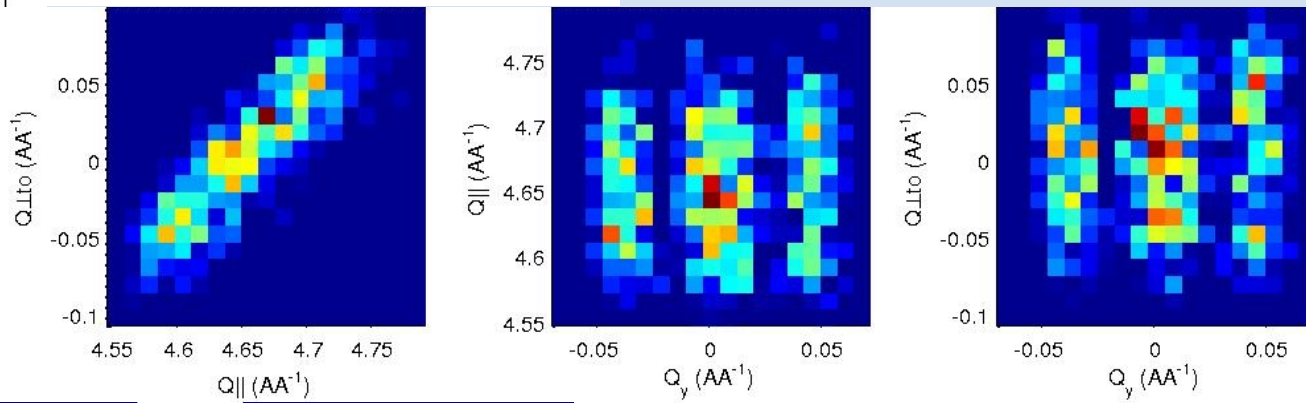

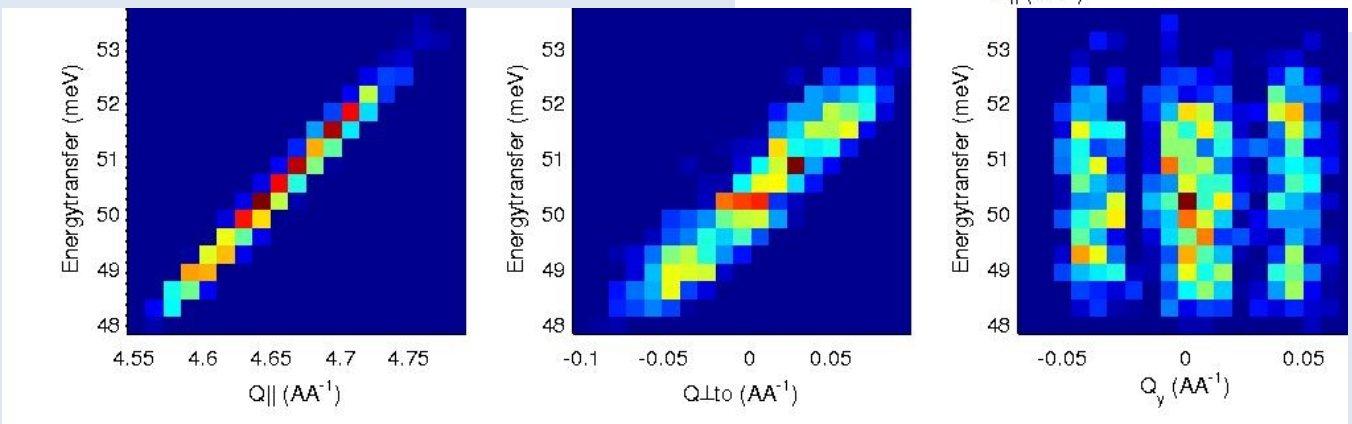

Getting simple things in a difficult way

$$\frac{dE}{E} = 2\frac{\tau}{\alpha L \lambda}$$

L_{pm}=50m L_{pm}=150m

τ_P=1ms

τ_P=2ms