A Monte Carlo simulation of Neutron Instrument Resolution Functions

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Outline

- A part of the 'Thermal Instrument Comparison Project'

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- An Introduction to the Resolution Function

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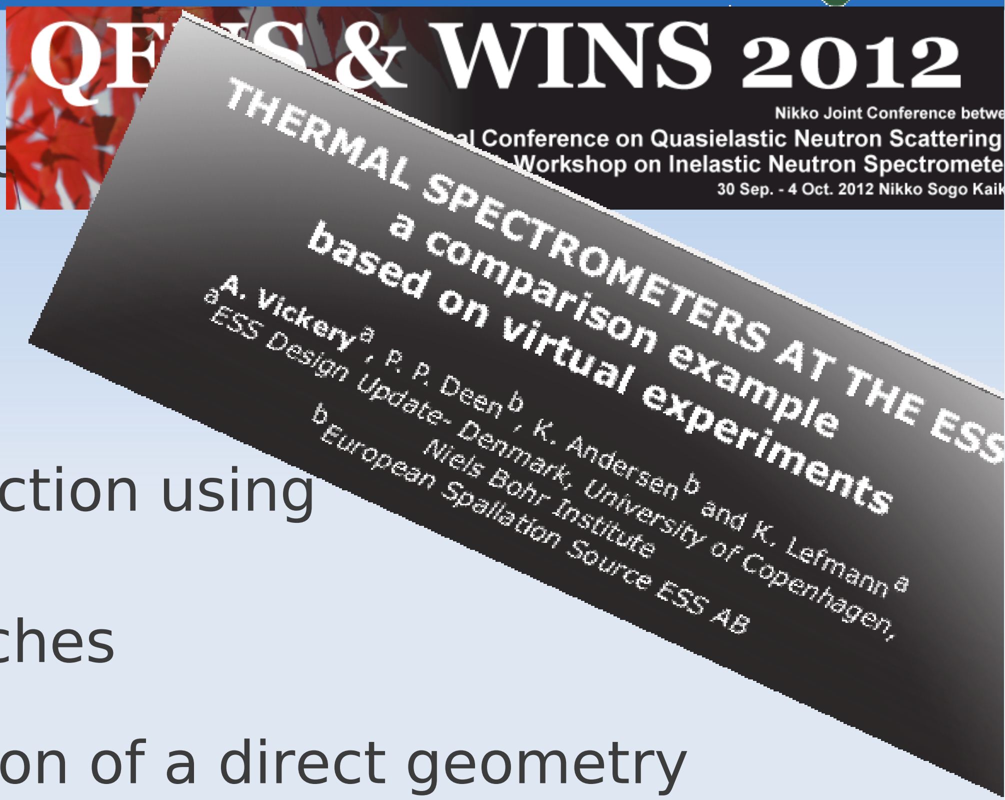

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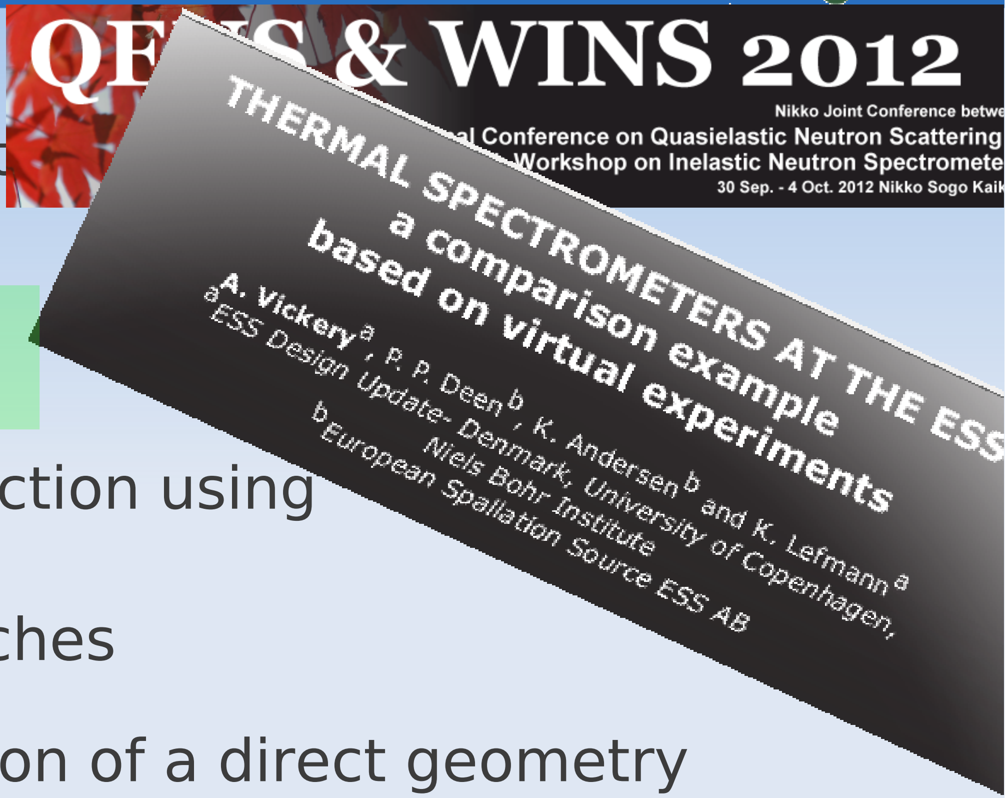

An introduction to the resolution function

- The resolution function defines the probability of detecting a neutron as function of $\Delta\mathbf{Q}$ (=$\mathbf{q}$ - $\mathbf{Q}$) and $\Delta\omega$ (=$\omega' - \omega$) when the instrument is set to measure the scattering process at ($\mathbf{Q}$,ω).

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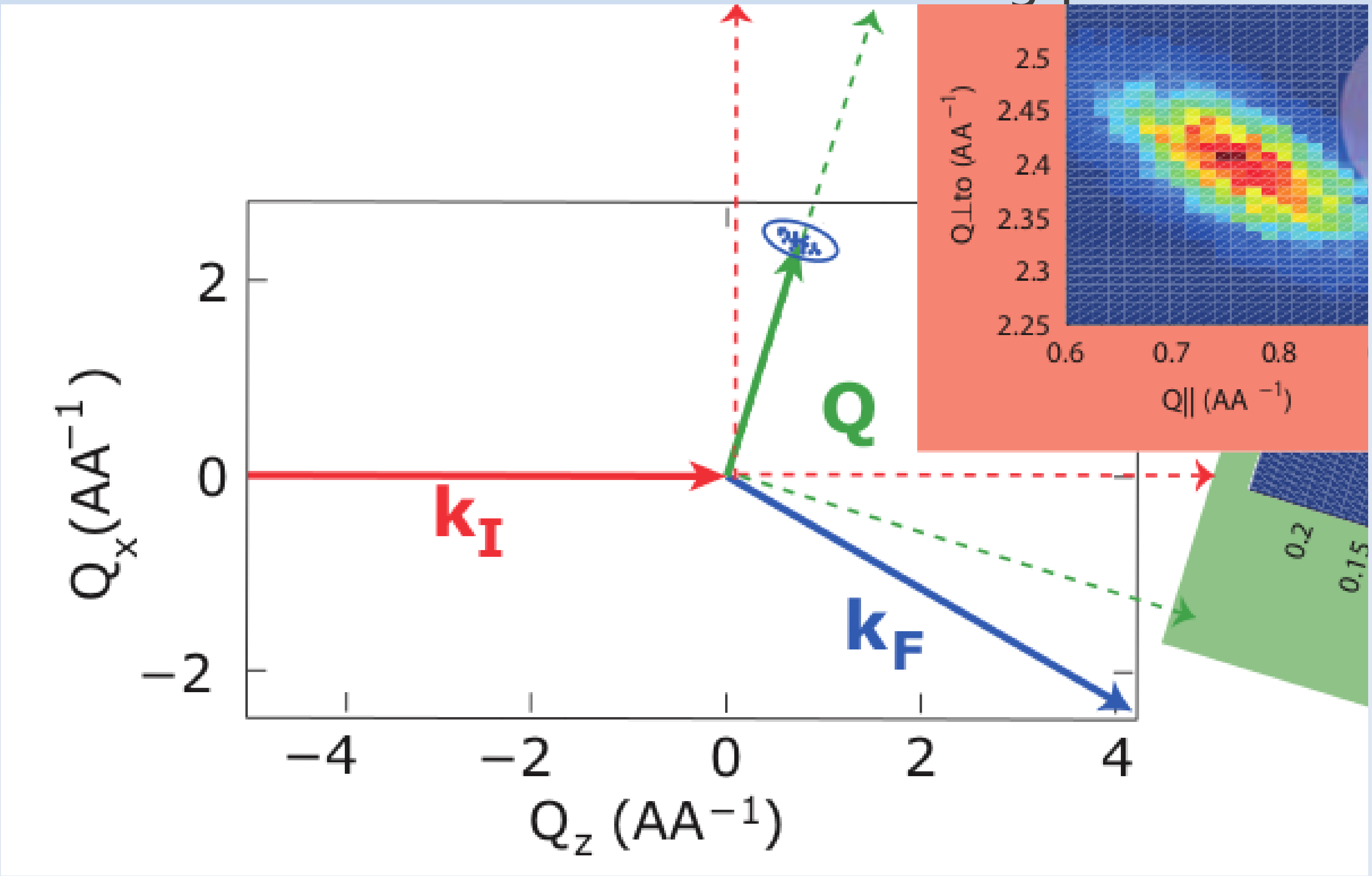

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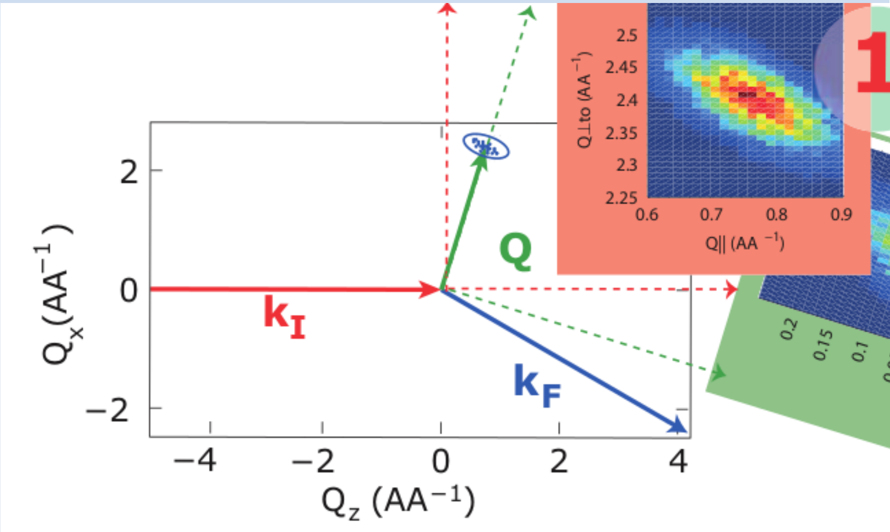
- The scattering profile obtained on a neutron scattering experiment is defined by the scattering function S (Q, ω). The intensity observed in a general experiment is related to the scattering function by the convolution integral



$$I_s(\mathbf{Q},\omega) = \iint R(\mathbf{q}-\mathbf{Q},\omega'-\omega)\, S(\mathbf{q},\omega')\, d\mathbf{q}\, d\omega'$$

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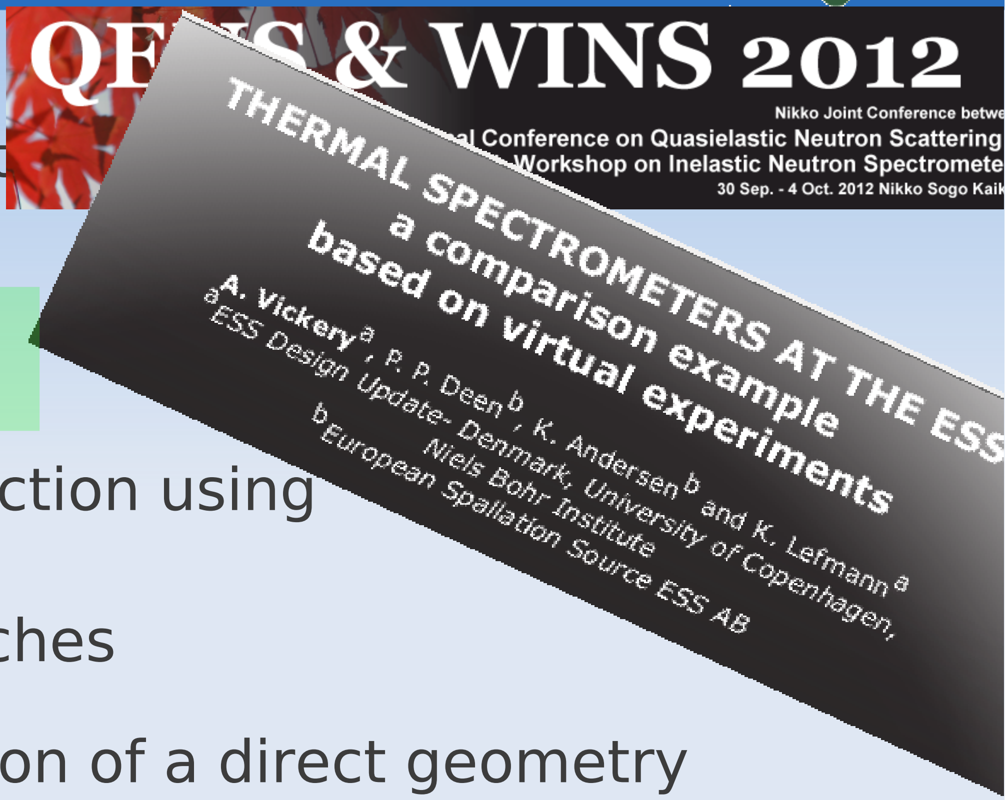

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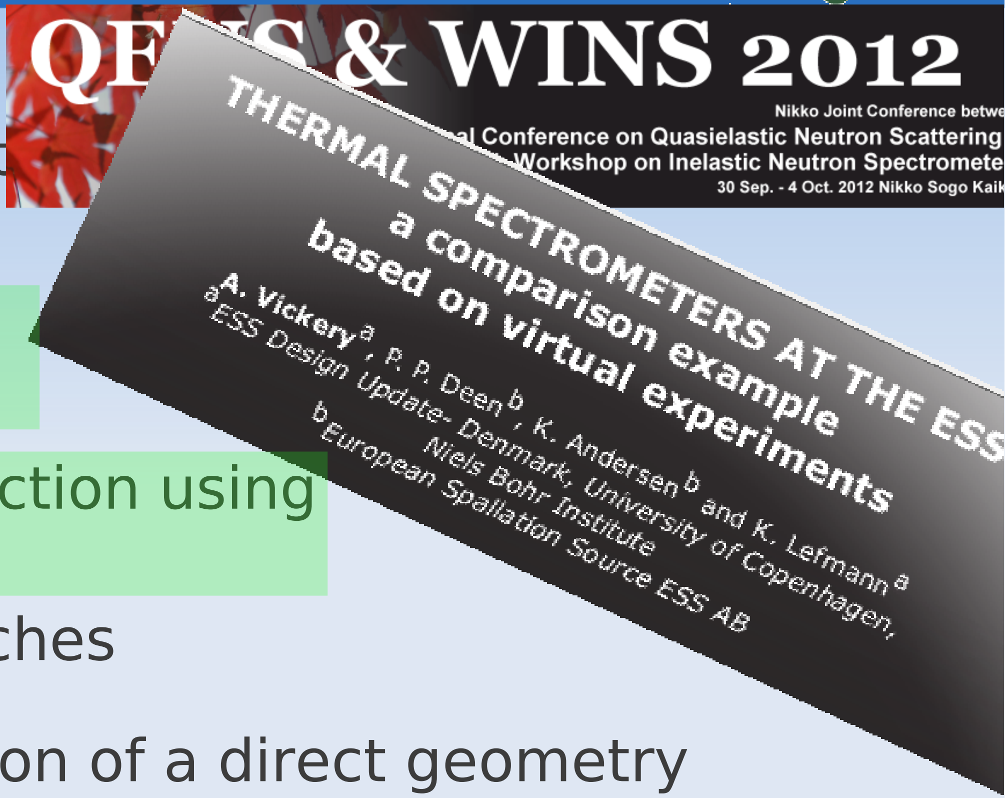

Calculation of the resolution function using McStas

- The resolution function defines the probability of detecting a neutron as function of Δ**Q** (=**q** - **Q**) and Δω (=ω' – ω) when the instrument is set to measure the scattering process at (**Q**,ω).
- The value of the resolution function at a given point in (**Q**, ω) space may be obtained by integrating the transmission probability P over all possible paths ($\mathbf{k}_i$, $\mathbf{k}_f$) to that point

$$R(\mathbf{Q}, \omega) = \int P(\mathbf{q}, \omega') \, \mathbf{dk}_\mathrm{i} \, \mathbf{dk}_\mathrm{f}$$

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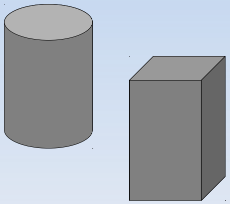
PROPORTIONAL TO THE SUM OF 'NEUTRON WEIGTHS'

Calculation of the resolution function using McStas

- Build a virtual copy of the instrument using the samples and monitor specialized for the calculation of a resolution function: **res_sample.comp** (for TAS) or **TOFRes_sample.comp** (for a t-o-f instrument) and **Res_monitor.comp**



- Both sample components are inelastic scatterers with completely uniform scattering in both solid angle and energy
- The scattered neutrons will have directions towards a given target (the analyzer for a TAS or a detector pixel for a direct geometry spectrometer).
- The detector stores in a file the individual initial and final neutron states, i.e. ($\mathbf{k}_i$, $\mathbf{k}_f$) along with the ***neutron weights***

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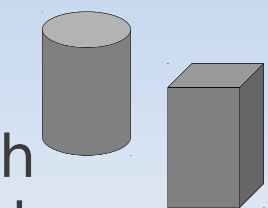

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- Whenever a neutron ray is recorded by the detector, the scattering event ($\mathbf{k}_{\mathbf{i, j}}$, $\mathbf{k}_{\mathbf{f, j}}$) and the associated neutron weight p_j (intensity) are written to a data file.
- From this file, the true value of the energy and momentum transfers can be calculated.
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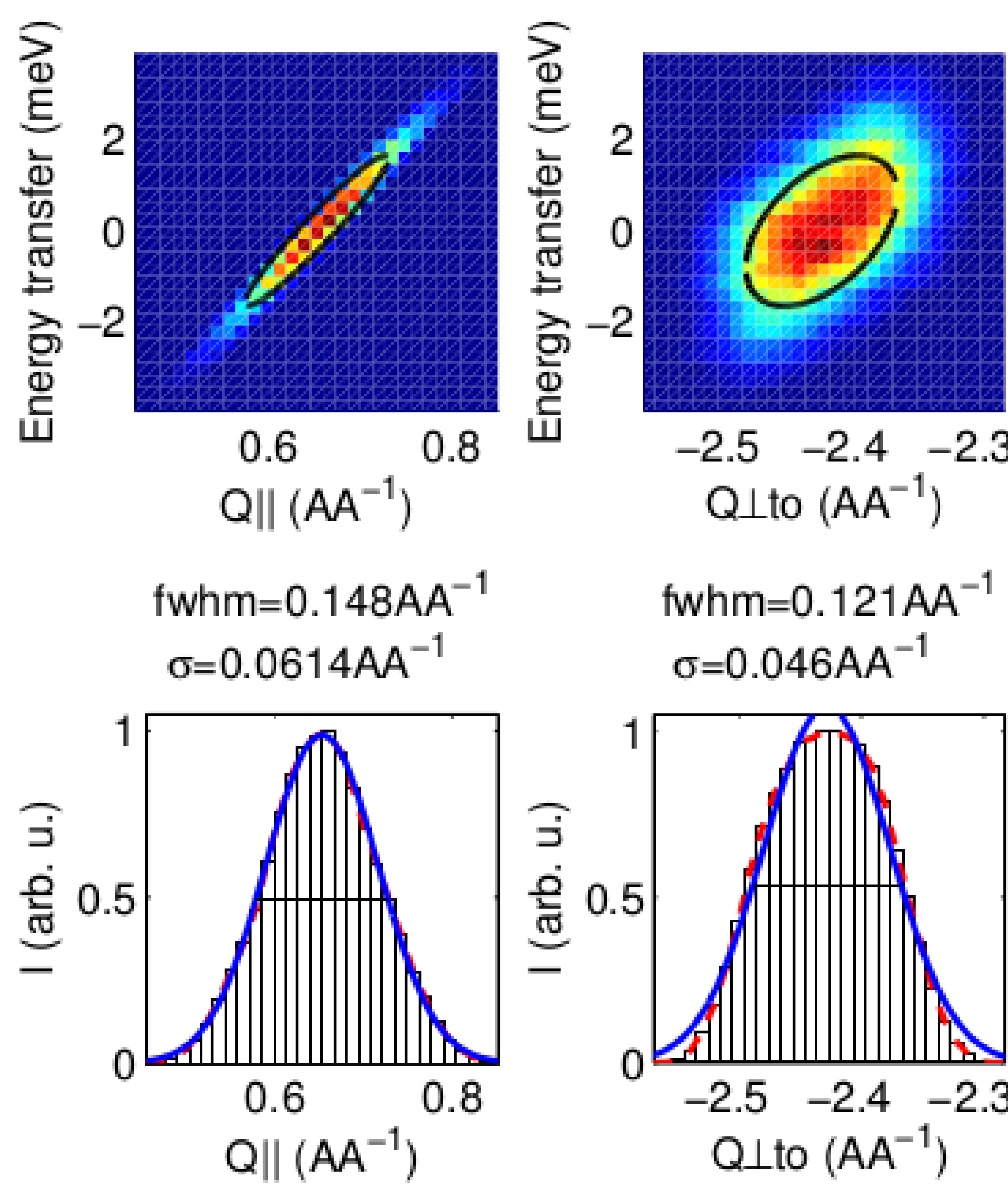

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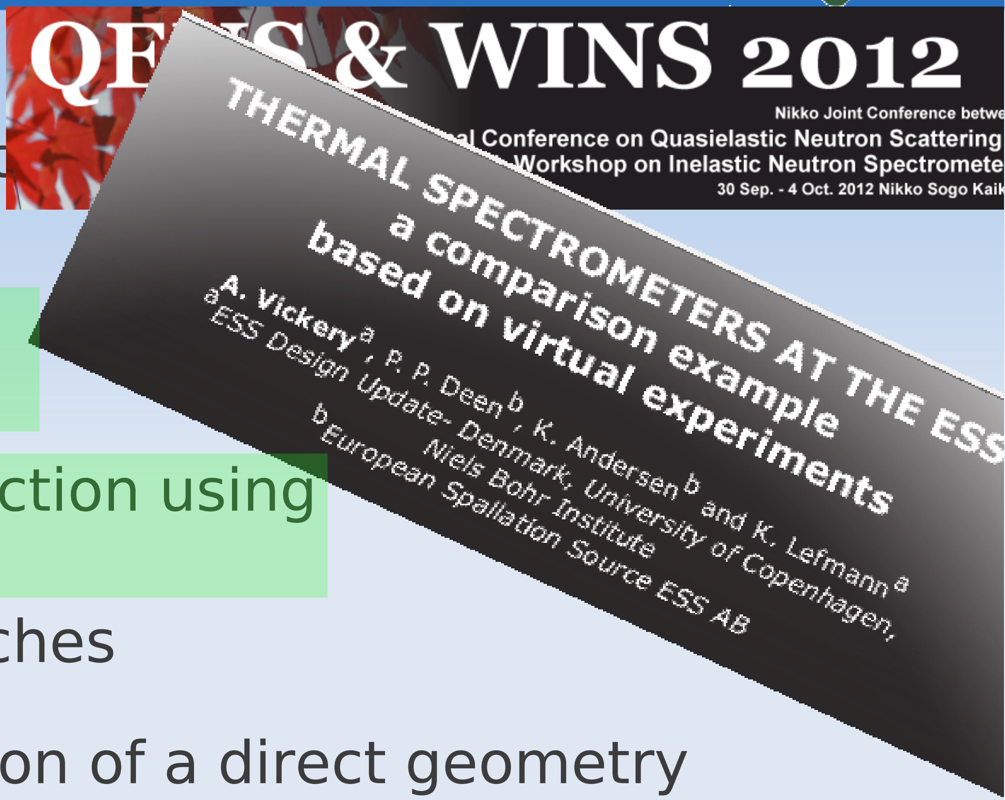

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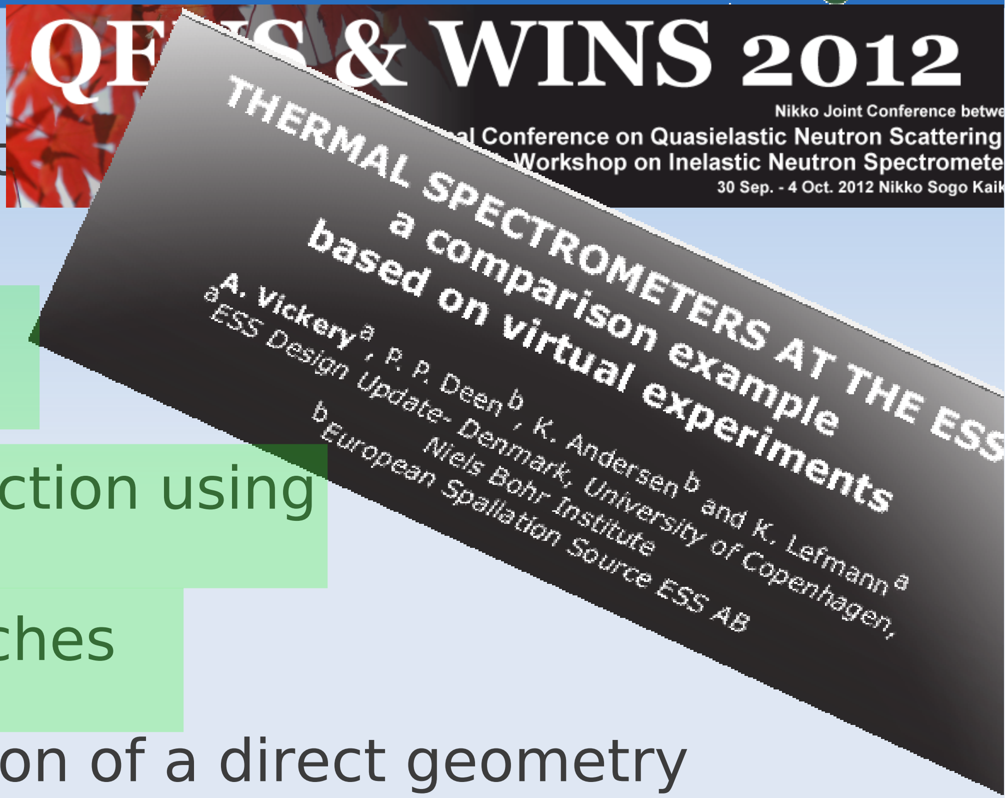
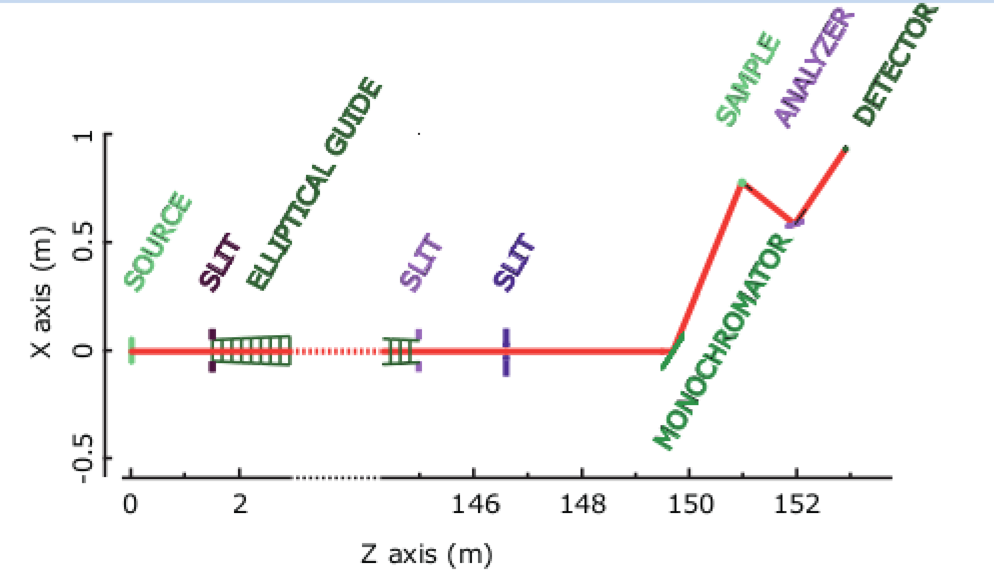


Comparison to analytical approaches

The resolution functions for two different instruments have been simulated and compared to results from analytical methods.



TRIPLE AXIS
SPECTROMETER

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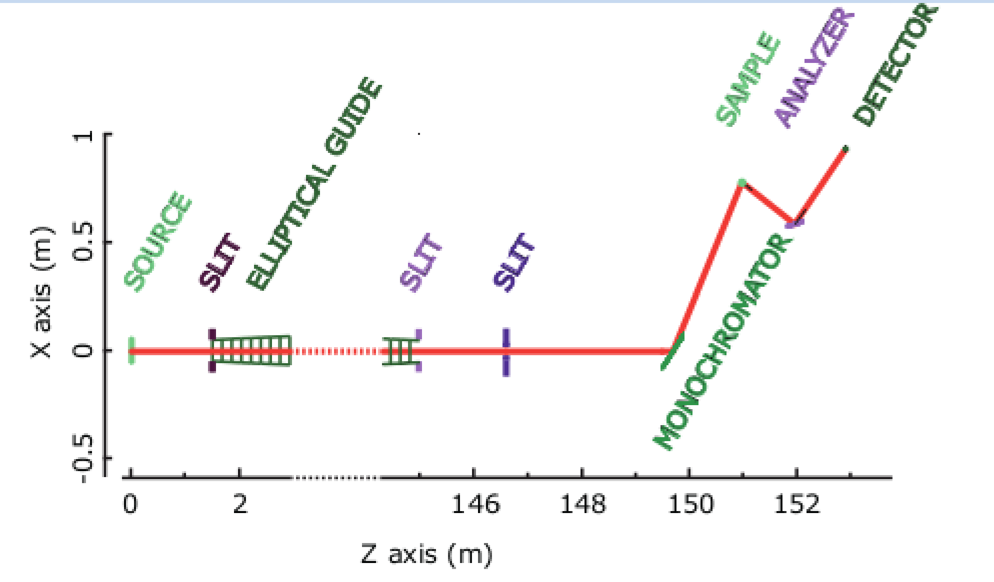
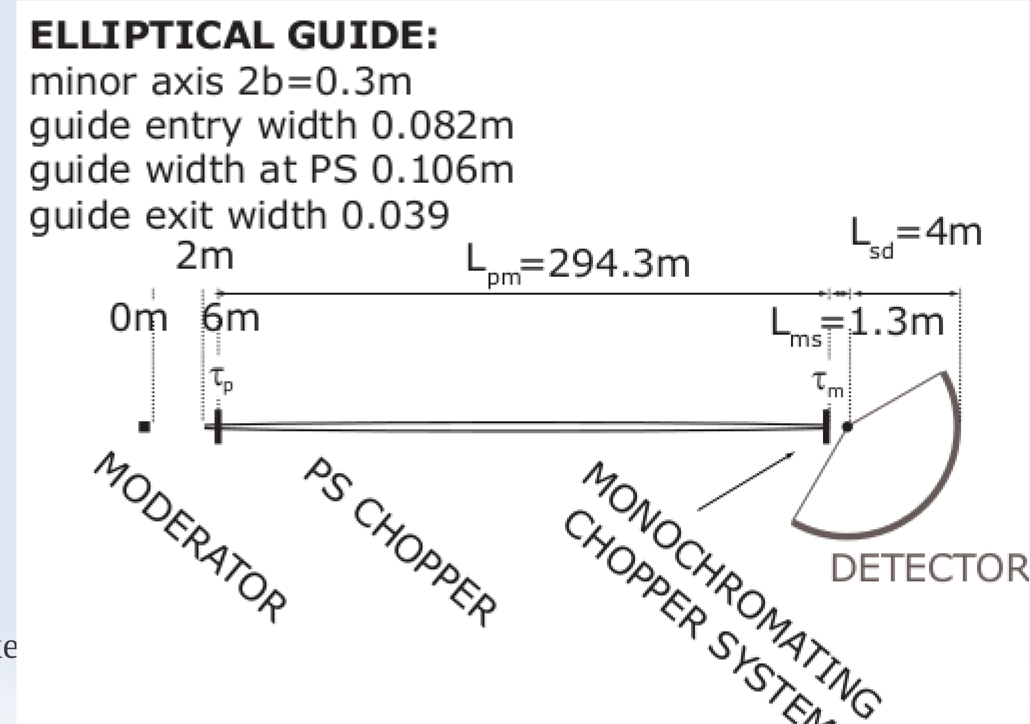


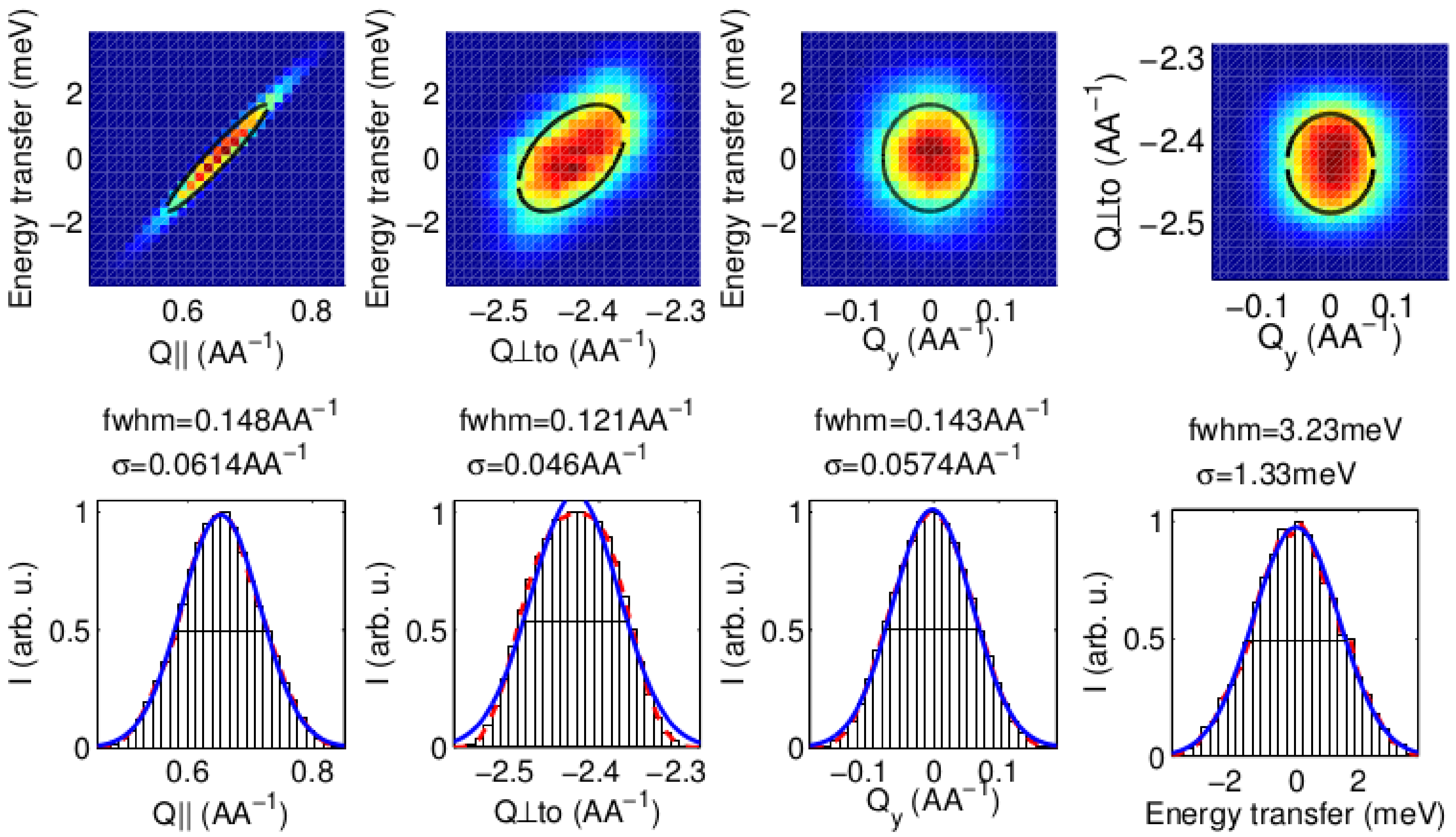
TRIPLE AXIS SPECTROMETER

DIRECT GEOMETRY TIME-OF-FLIGHT SPECTROMETER



Comparison to analytical approaches

The resolution function of a direct geometry chopper spectrometer simulated with the McStas package at a scattering angle of 30.14◦ and EI = EF = 48.45 meV. The sample is a hollow cylinder of height 2 cm and inner/outer radii of 2.5 mm/5 mm. The blue curves are Gaussian fits to the data, from which the full widths at half maximum (fwhm's) are derived. The detector pixel of size (55 × 105) mm2 (h×v) is at a distance of 4 m from the sample. The width of the time bin is 1μs. The black contours are analytical results.



Comparison to analytical approaches

- The simulated results are compared to analytical results from the ResLib package (MATLAB based) and calculations by Nicoló Violini and Jörg Voigt.

- The simulated results were in agreement with the results obtained with analytical methods

- For the direct geometry Chopper Spectrometer, the linewidths in Q agree within 5% and the linewidths in E agree within 3%

- For the Triple Axis Spectrometer, the energy- and transverse Q-resolution agree within a 2%, whereas the parallel and vertical Q-resolution agrees within 20%

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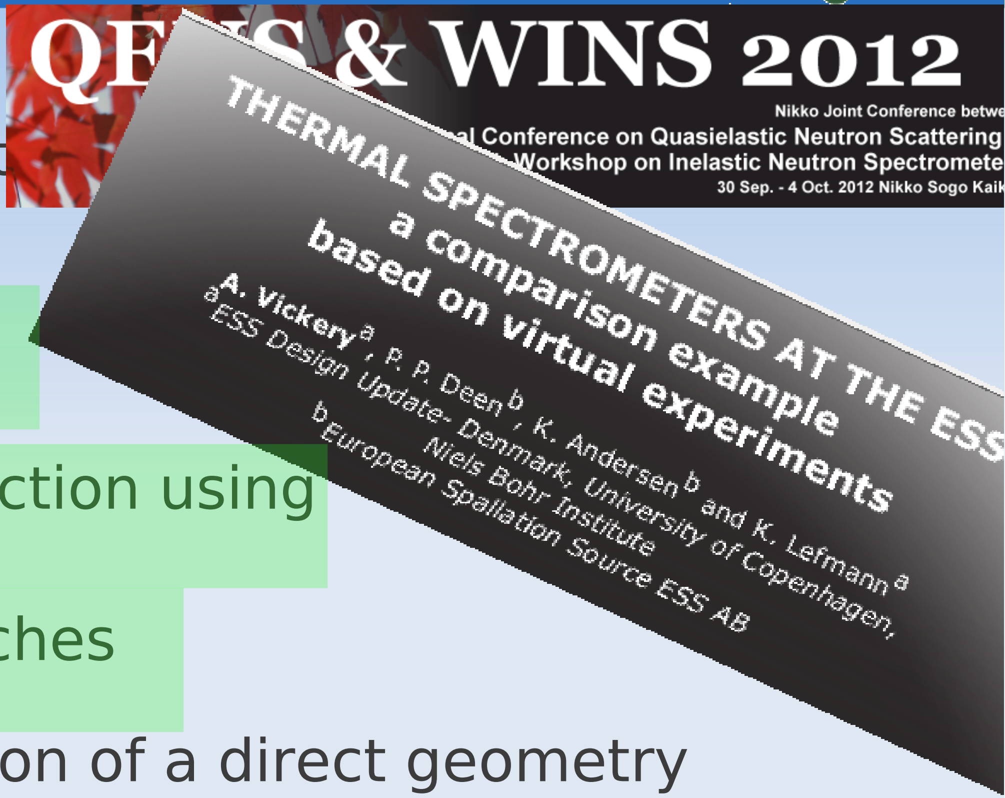

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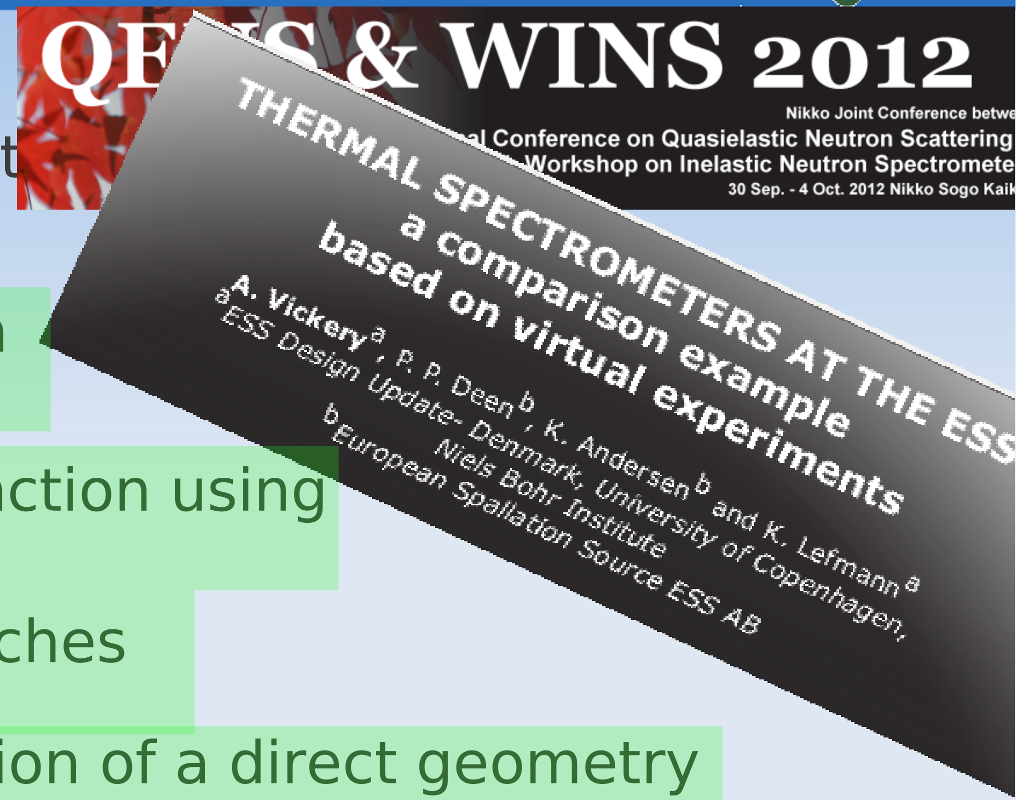
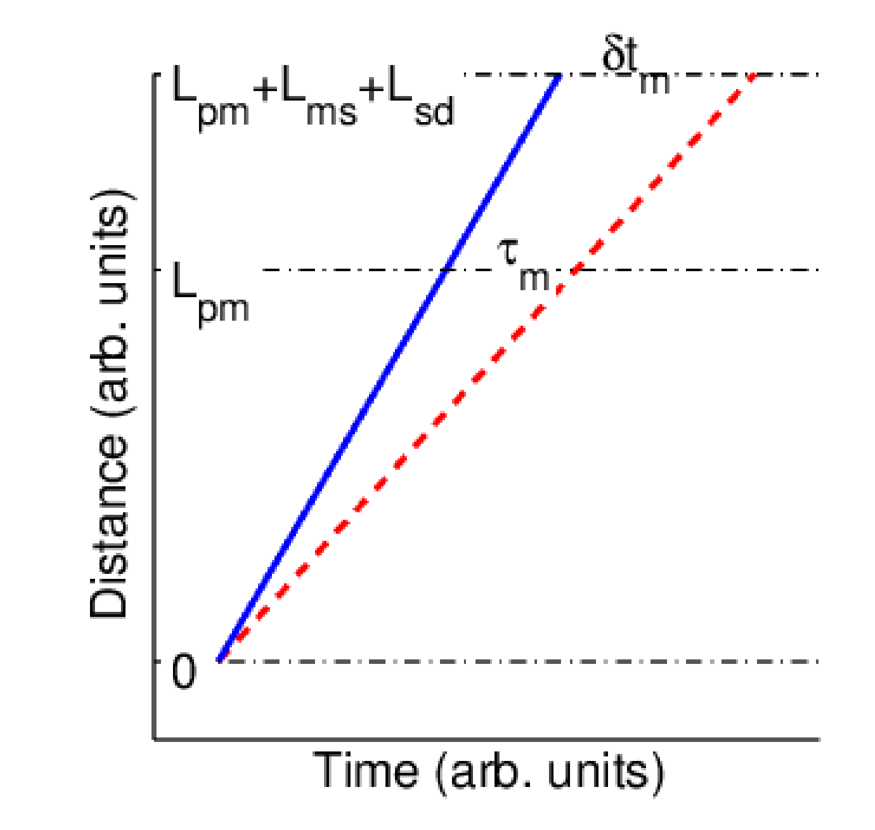


EXAMPLE: energy resolution of a direct geometry chopper spectrometer



$$\frac{\delta t_{\rm m}}{L_{\rm pm}+L_{\rm ms}+L_{\rm sd}} = \frac{\tau_{\rm m}}{L_{\rm pm}}$$

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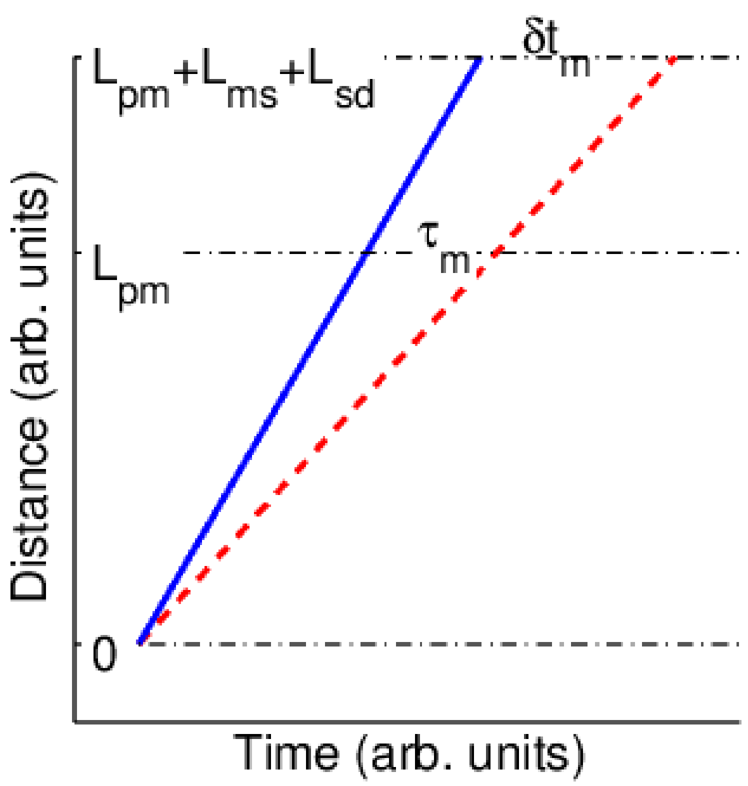

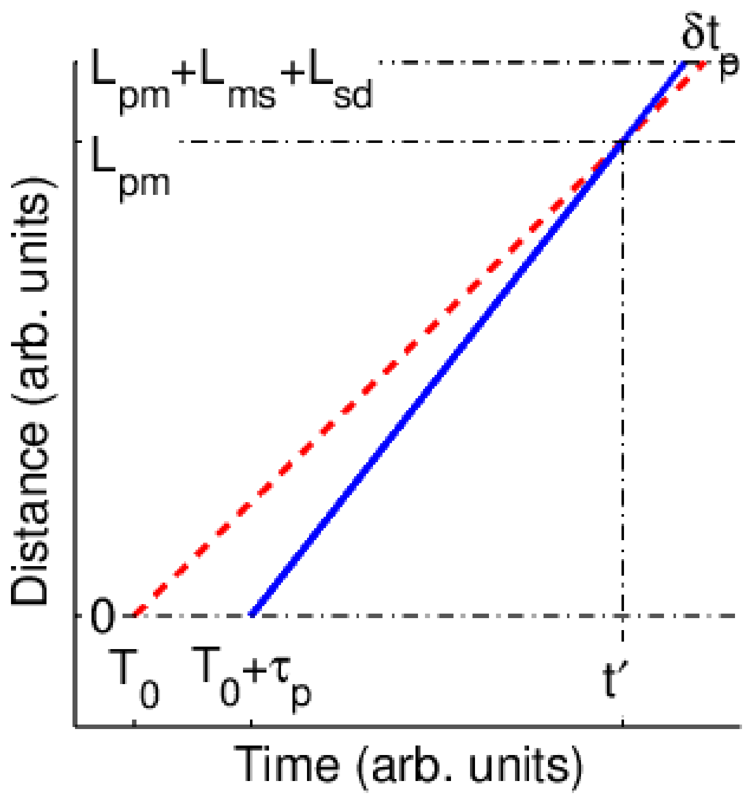

$$\frac{\delta t_{\rm m}}{L_{\rm pm}+L_{\rm ms}+L_{\rm sd}}=\frac{\tau_{\rm m}}{L_{\rm pm}}$$

$$\frac{\delta t_{\rm p}}{L_{\rm ms}+L_{\rm sd}}=\frac{\tau_{\rm p}}{L_{\rm pm}}\,.$$

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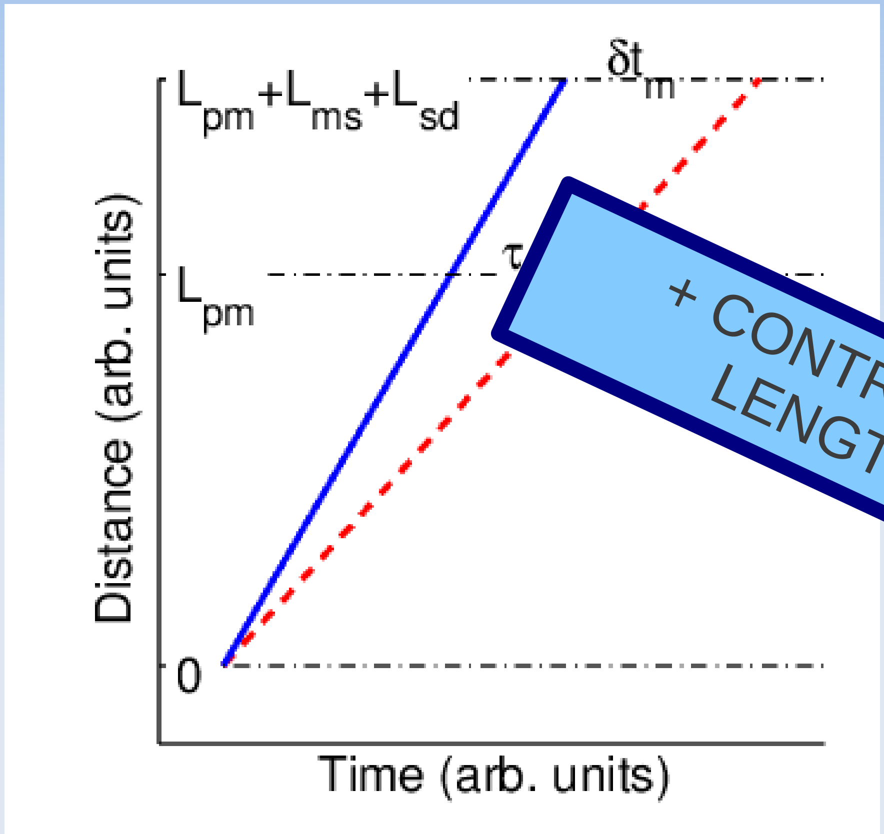

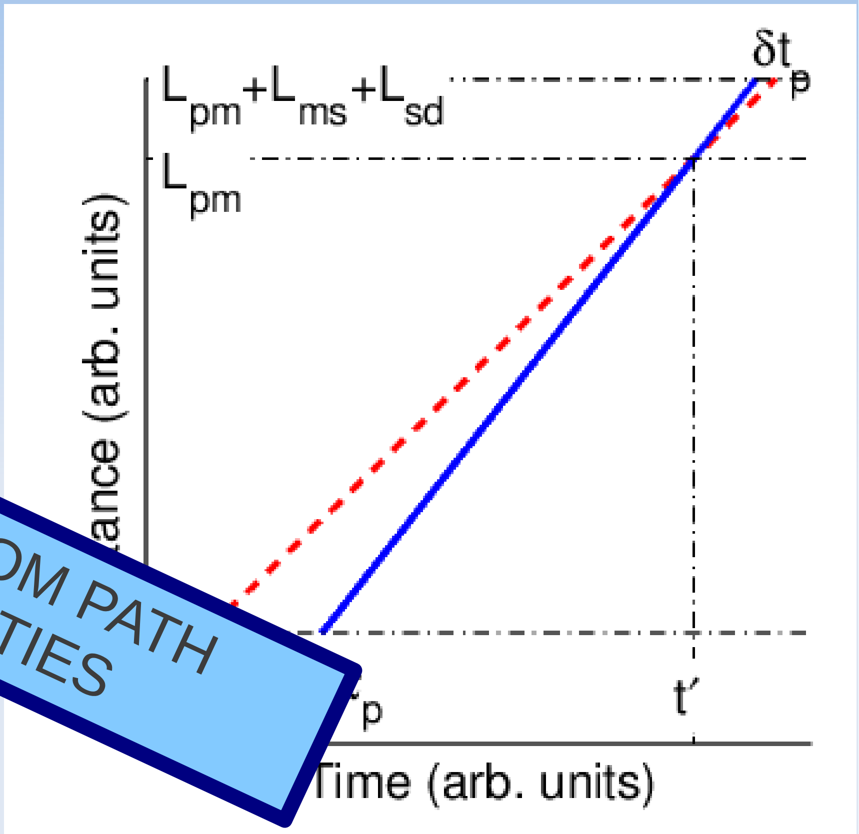

+ CONTRIBUTIONS FROM PATH LENGTH UNCERTAINTIES

$$\frac{\delta t_{\mathrm{m}}}{L_{\mathrm{pm}} + L_{\mathrm{ms}} + L_{\mathrm{sd}}} = \frac{\tau_{\mathrm{m}}}{L_{\mathrm{pm}}}$$

$$\frac{\delta t_{\mathrm{p}}}{L_{\mathrm{ms}} + L_{\mathrm{sd}}} = \frac{\tau_{\mathrm{p}}}{L_{\mathrm{pm}}} .$$

EXAMPLE: energy resolution of a direct geometry chopper spectrometer

Using $E = h^2/(2m\lambda^2)$ and $t = mL\lambda/h$

the energy width at the detector amounts to

$$\sigma_E = \sigma_t \frac{h^3}{m^2\,\lambda^3\,L_{\mathrm{sd}}}$$

The magnitude of σ_t , ***the standard deviation*** of the final detected time pulse, is estimated by adding in quadrature the time spread contributions from the two chopper pairs and the path length uncertainty $\sigma_L \approx 5$ mm. The fwhm energy width is then estimated as $\Delta E = 2.35\sigma_E$

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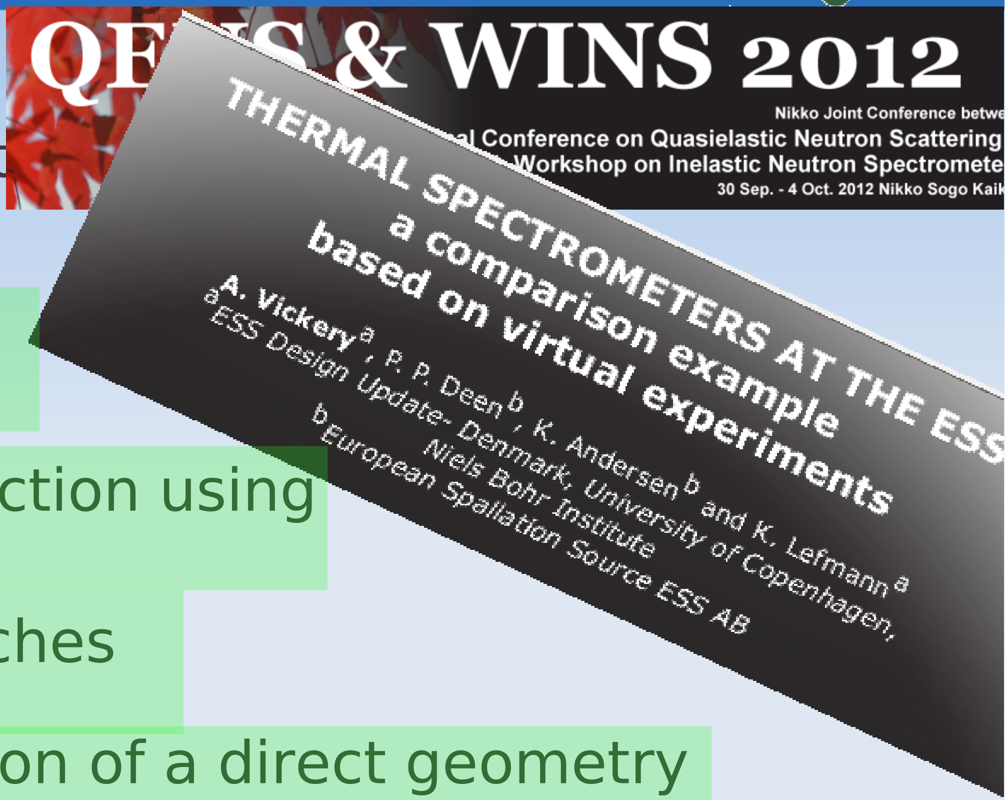

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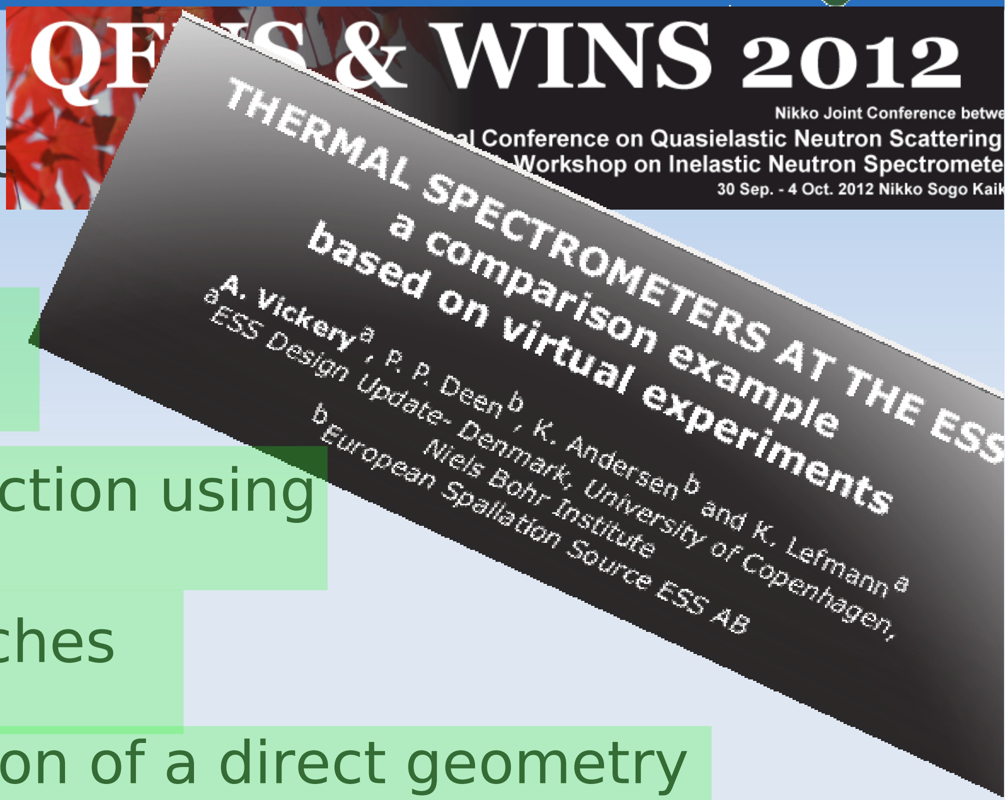

CONCLUSION

- The McStas simulation package is a useful tool *also* for the simulation of instrument resolution functions
- the simulated results were in agreement with the results obtained with analytical methods
- it is now possible to perform detailed Monte Carlo simulation of a complex neutron scattering instrument within a tolerable time (few seconds –minutes)
- we believe that the use of simulations should be expanded from the design phase of an instrument to directly support the user community
- The simulation of an instrument resolution function at a particular point in (Q, ω) space is just one example of simulation-aided decision support
- To be successful, it is of crucial importance that the simulation tools are implemented with great care and the virtual instrument is maintained as careful as the real instrument