HELMHOLTZ ZENTRUM BERLIN
für Materialien und Energie

Upgrade of the cold three-axis spectrometer FLEX at BER II

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Klaus Habicht
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McStas ICNS 2009 satellite workshop
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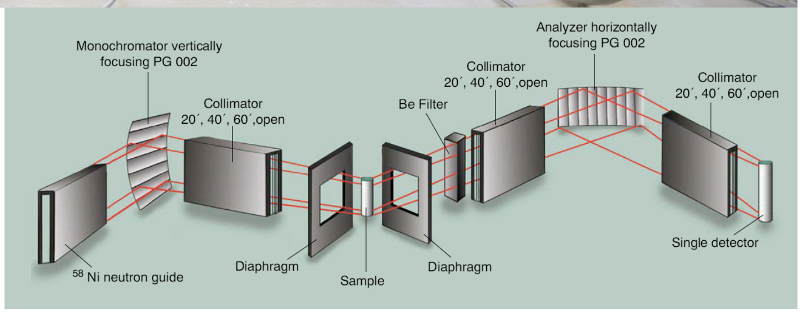
Acknowledgements

F. Mezei	LANL, USA
C. Pappas	HZB, Germany
A. Tennant	HZB, Germany
T. Krist	HZB, Germany

Outline of Talk:

Introduction	Current FLEX operation
	General layout of upgraded FLEX
Monte Carlo	Independent checks on the validity of MC method
	Simulations on FLEX's primary spectrometer
Conclusions	

Current FLEX – usual operation



low energy excitations in:

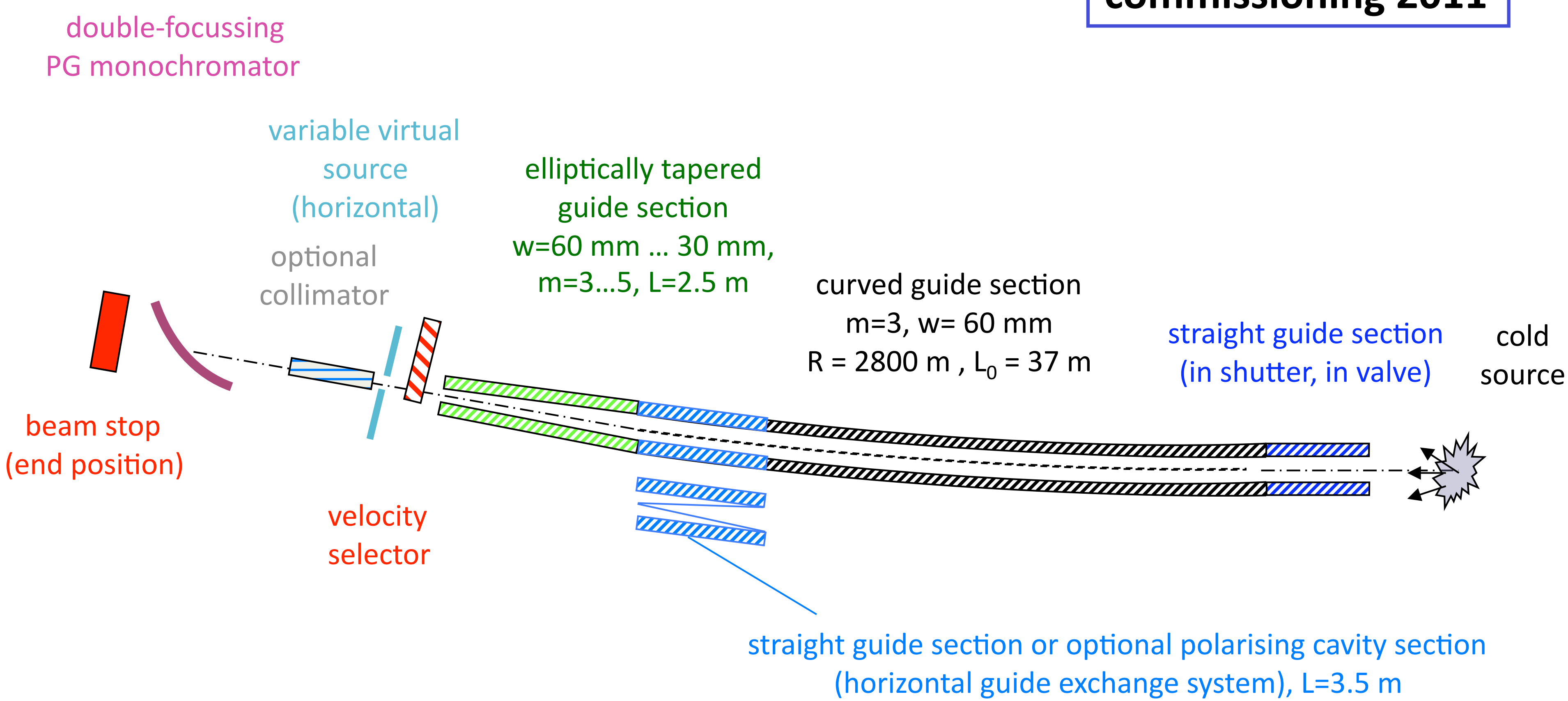
- quantum magnetism
- high-T_c superconductors
- heavy fermions

experimental need for:

- good signal to noise
- high intensity
- but moderate wavevector resolution

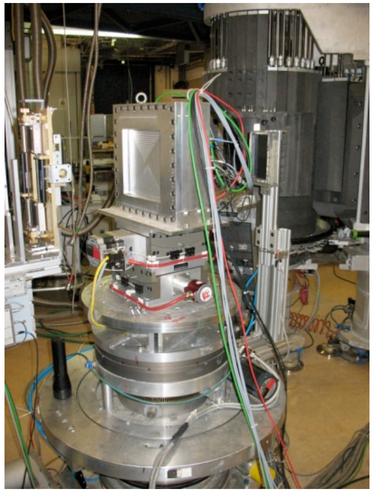
Upgraded FLEX – primary spectrometer layout

commissioning 2011

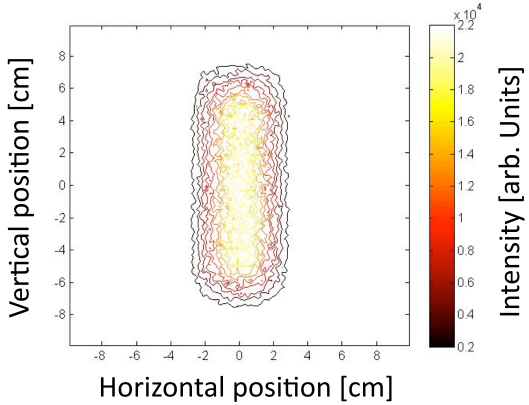


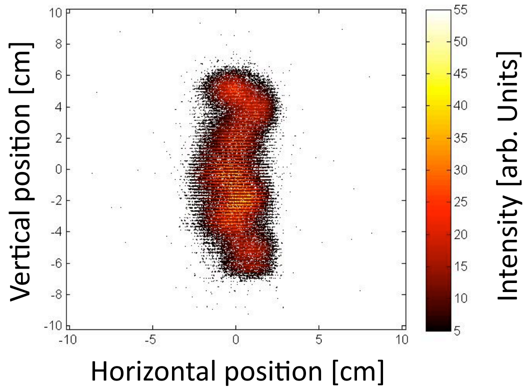
Checks of Monte Carlo validity: PSD measurements

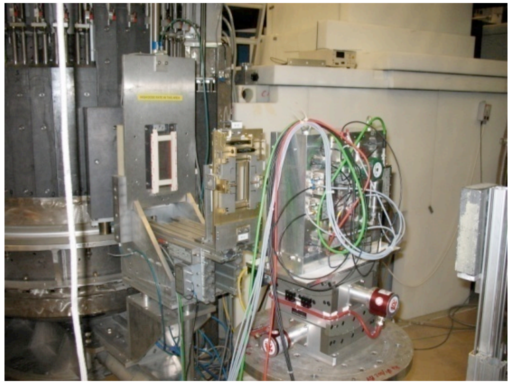
- sample position measurements at FLEX directly compared with Vitess simulations
- checked at various wavelengths and monochromator focusing radii

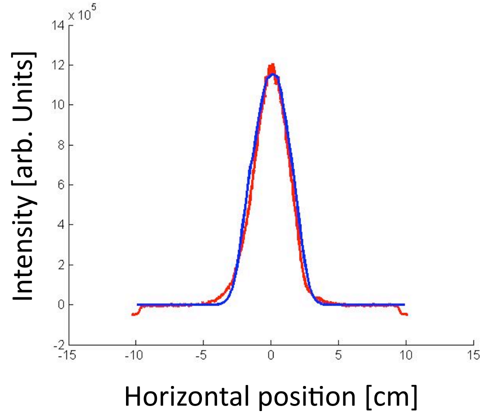


k_I = 1.55 Å^{-1} with flat monochromator









Checks of Monte Carlo validity: PSD measurements

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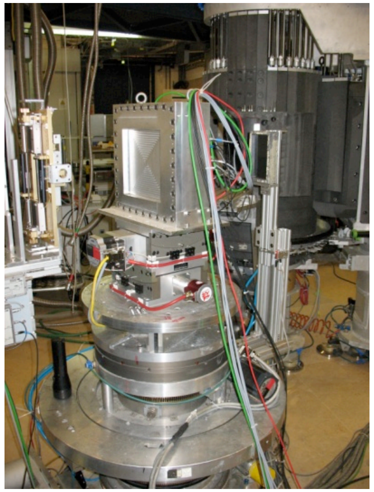
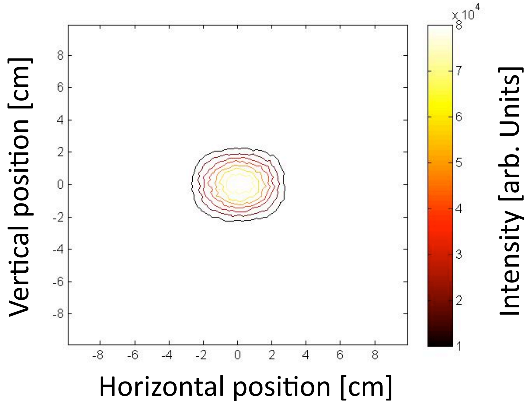
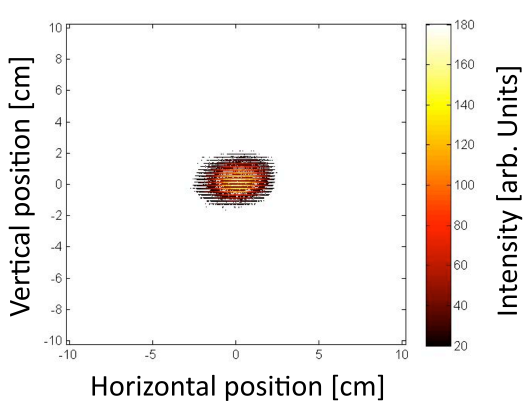
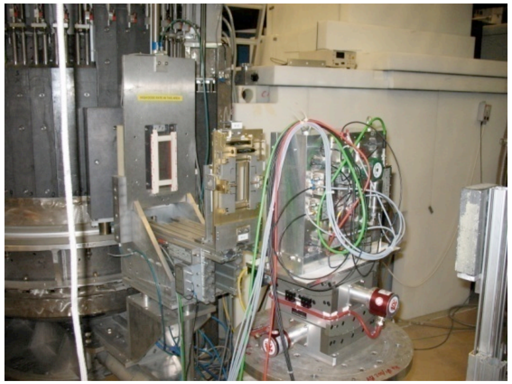
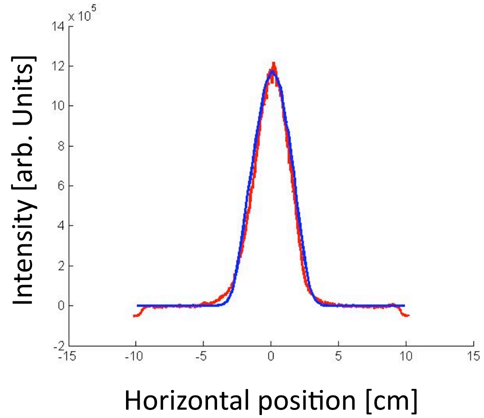


k_I = 1.55 Å^{-1} with vertically focused monochromator



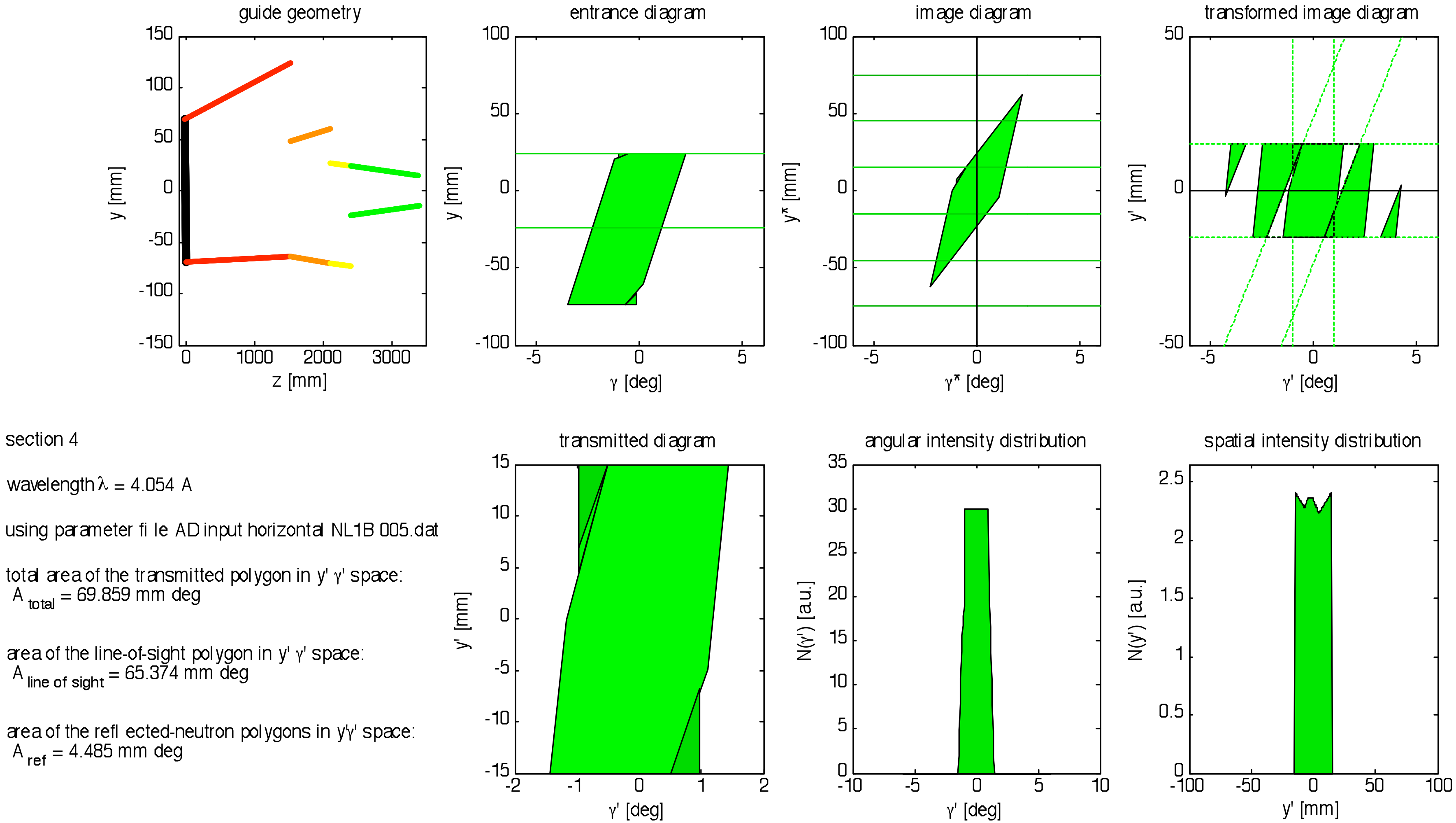






Checks of M.C. validity: acceptance diagrams

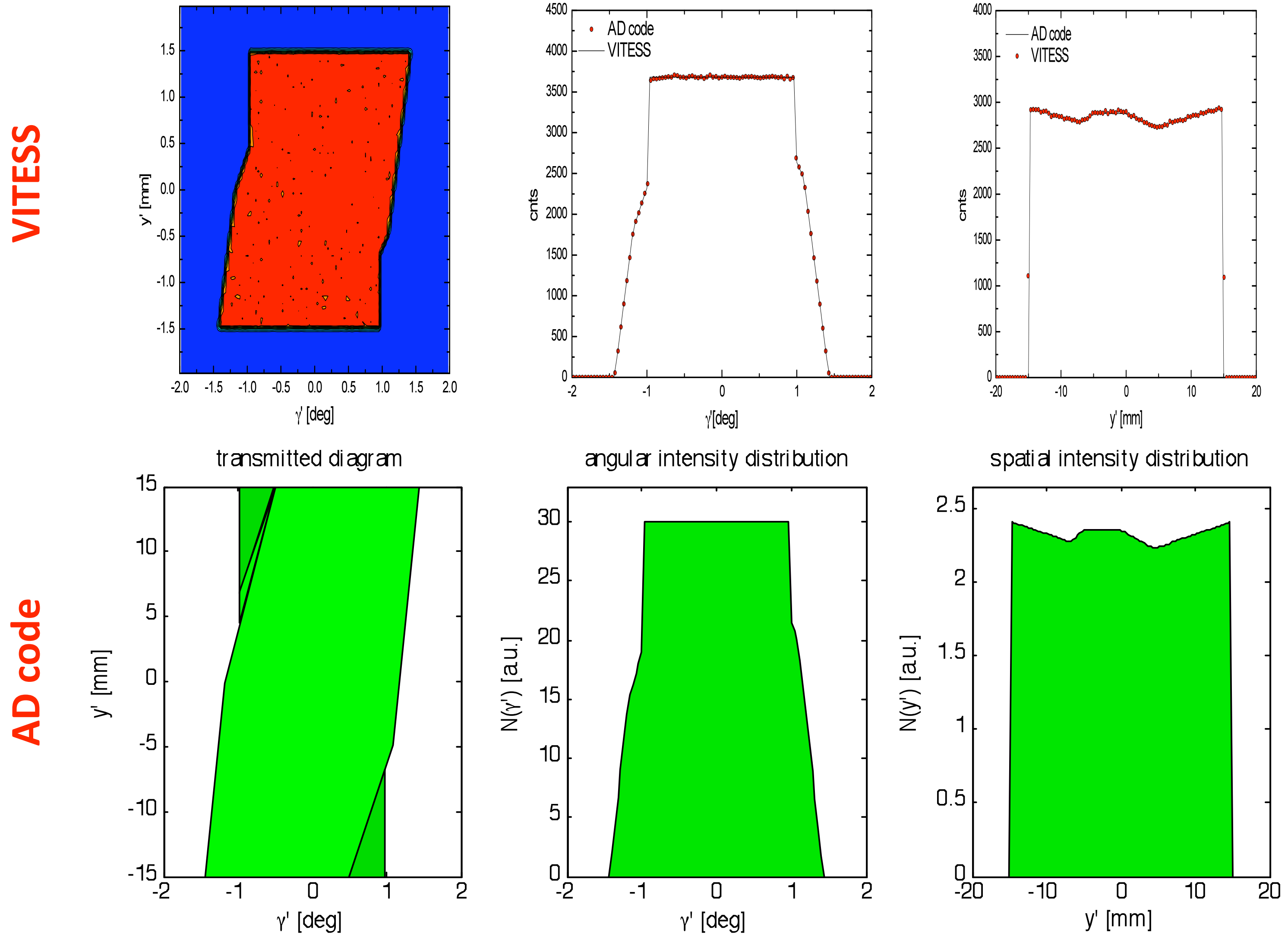
- acceptance diagrams of horizontal status of current FLEX guide (NL1b) at in-pile section



J.R.D. Copley, NIM **287**, 363 (1990)

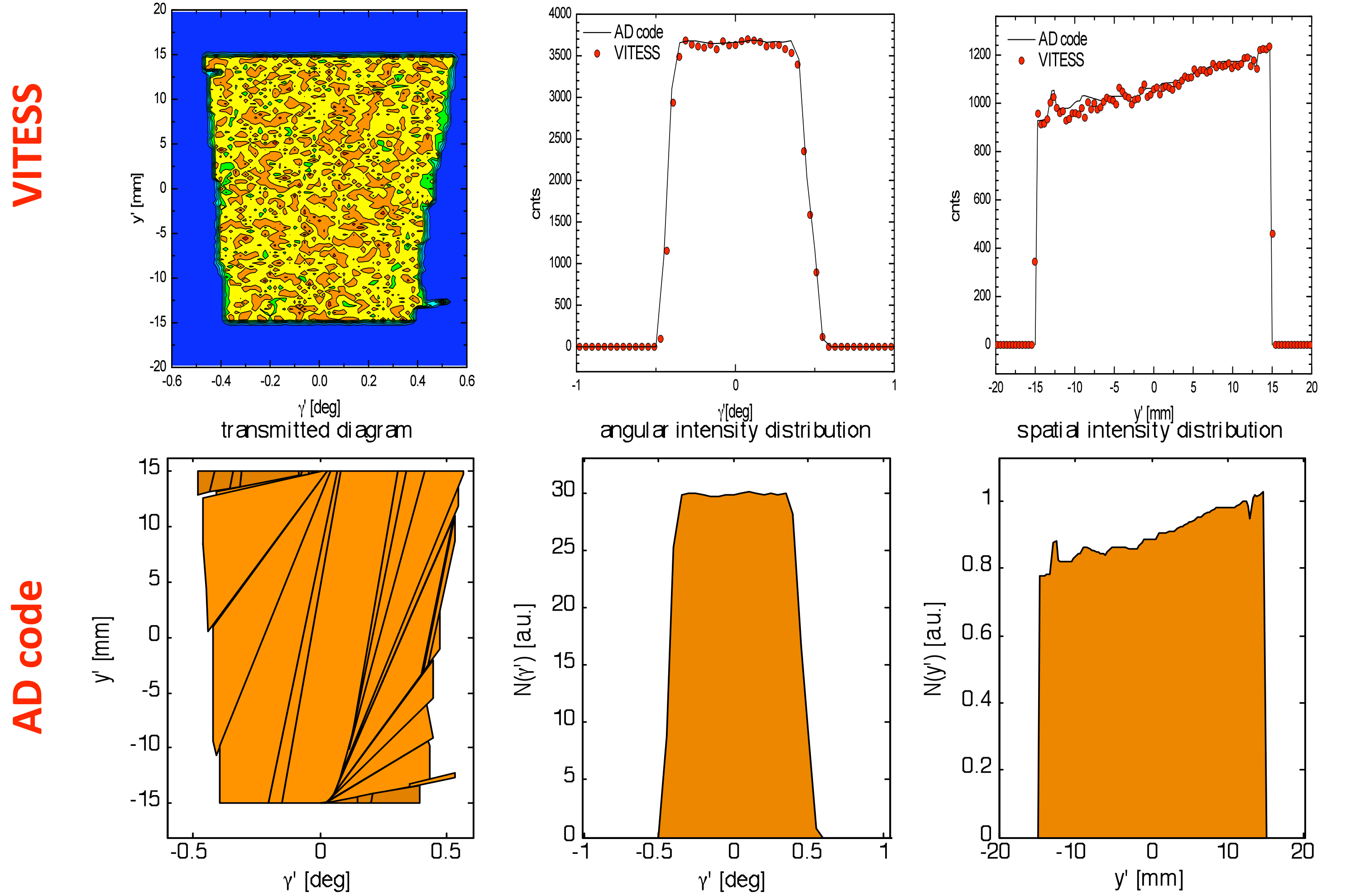
Checks of M.C. validity: acceptance diagrams

- A.D. at the current in-pile section directly compared to Vitess M.C. simulations



Checks of M.C. validity: acceptance diagrams

- A.D. half way through FLEX's curved guide directly compared to Vitess M.C. simulations

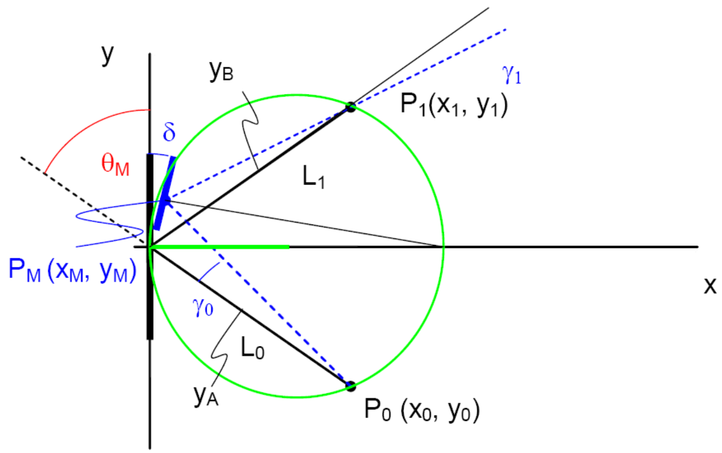


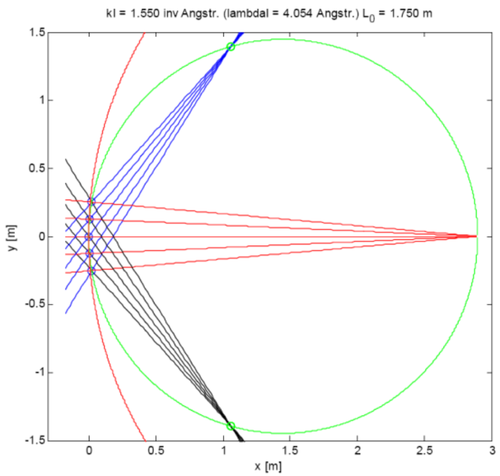
- test for Vitess code but also very helpful in checking the model parameters

Checks of M.C.: virtual source-monochromator

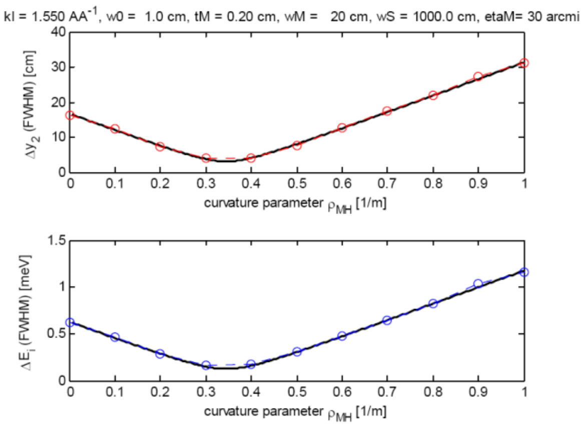
- McStas simulations versus the analytical Popovici model - widths

virtual source geometry – symmetric case

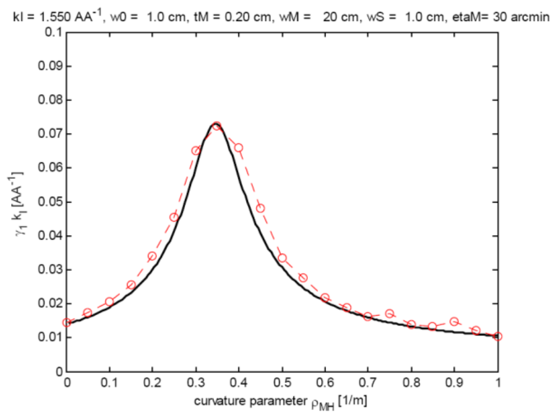




Spatial and monochromatic focusing



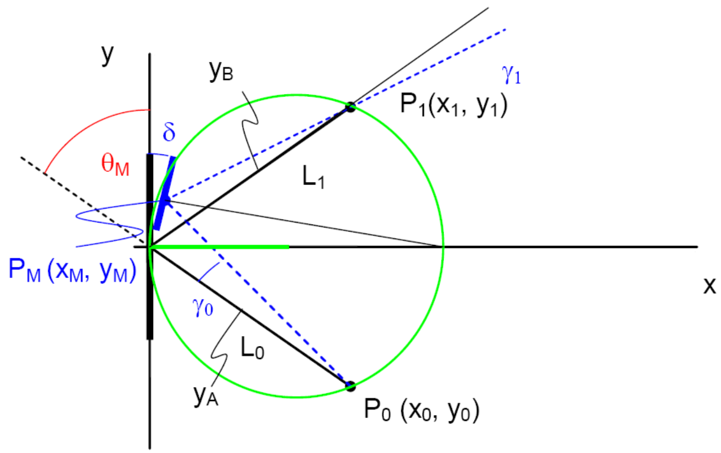
Width of transverse incident wavevector in scattering plane

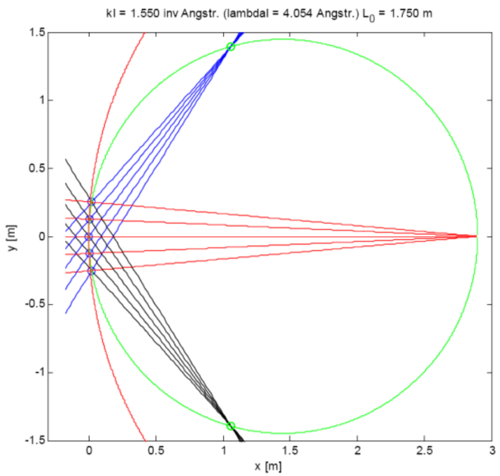


Checks of M.C.: virtual source-monochromator

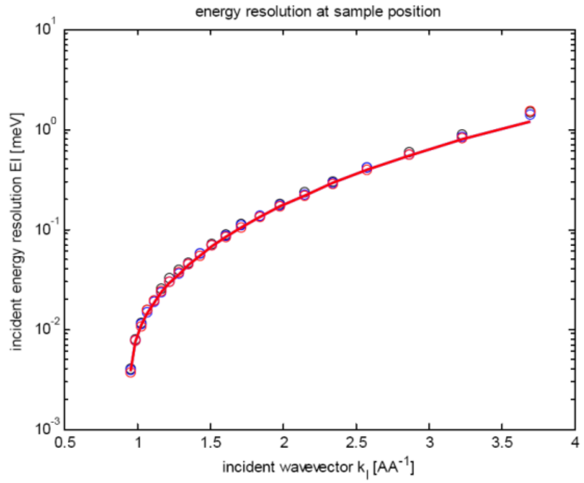
- McStas simulations versus the analytical Popovici model - widths

virtual source geometry – symmetric case

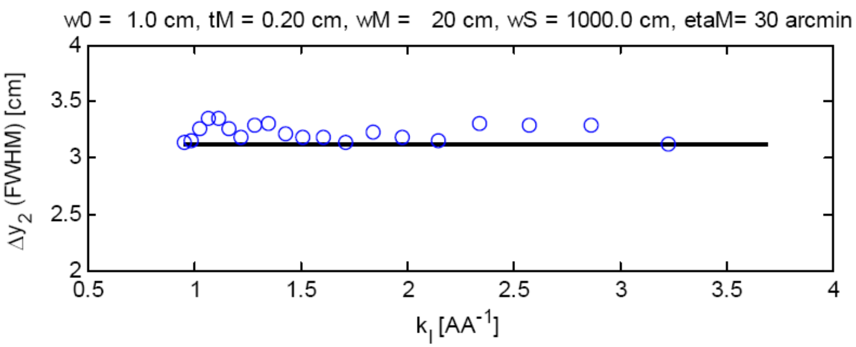




Wavevector dependence of energy width



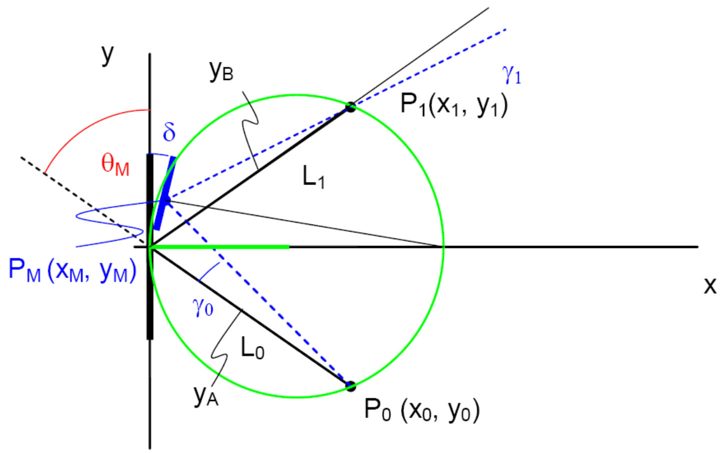
Wavevector dependence of horizontal spot size

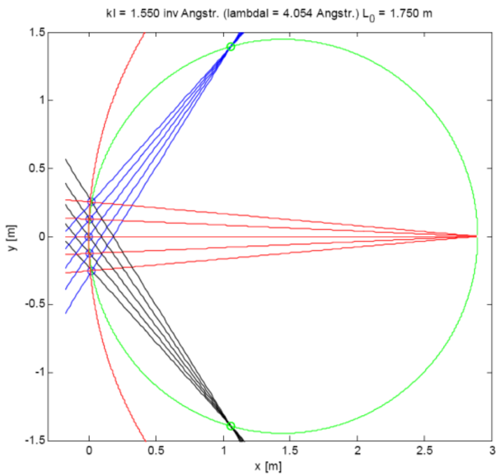


Checks of M.C.: virtual source-monochromator

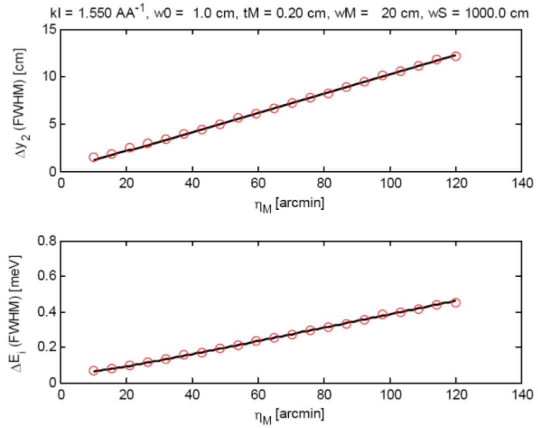
- McStas simulations versus the analytical Popovici model - widths

virtual source geometry – symmetric case

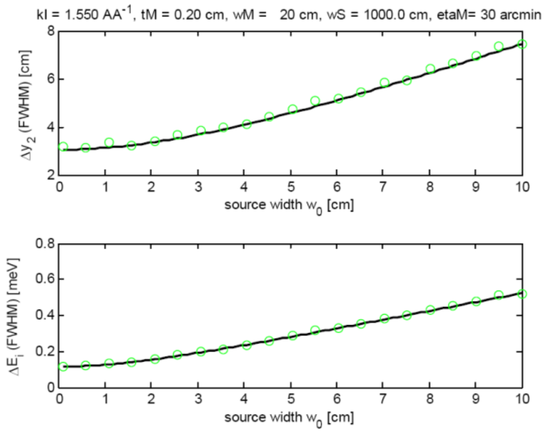




Mosaicity dependence of horizontal spot size and ΔE



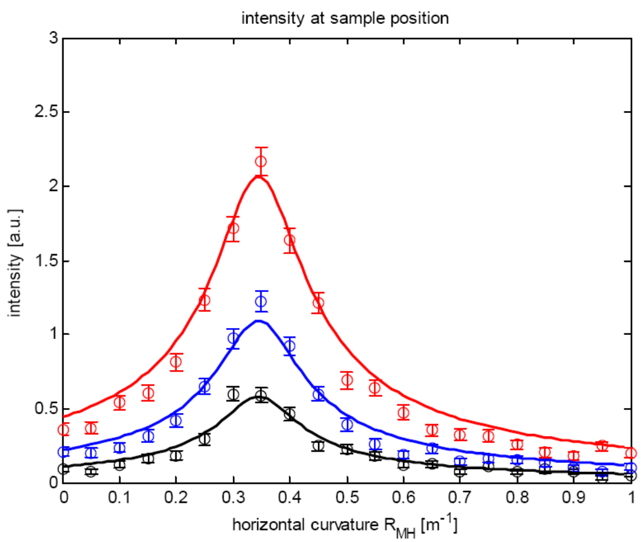
Source width dependence of horizontal spot size and ΔE



Checks of M.C.: virtual source-monochromator

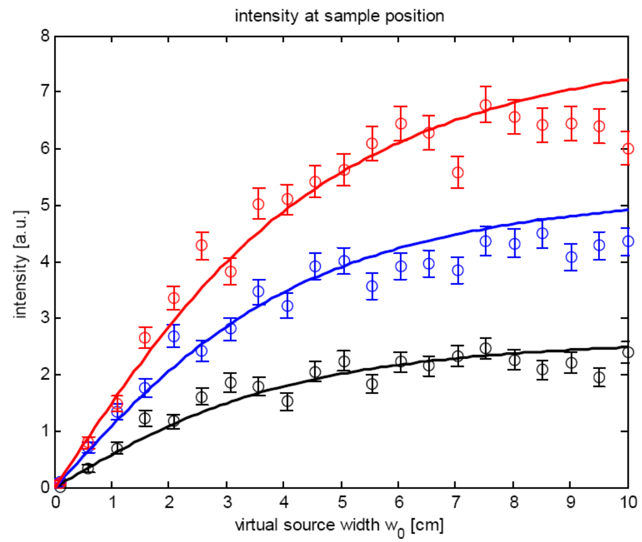
- McStas simulations versus the analytical Popovici model - intensities

Intensity as a function of horizontal focusing



virtual source width w0=2 cm, sample width wS=2 cm
w0=1 cm wS=2 cm
w0=1 cm wS=1 cm

Intensity as a function of virtual source width



monitor width at the sample position:
3 cm
2 cm
1 cm

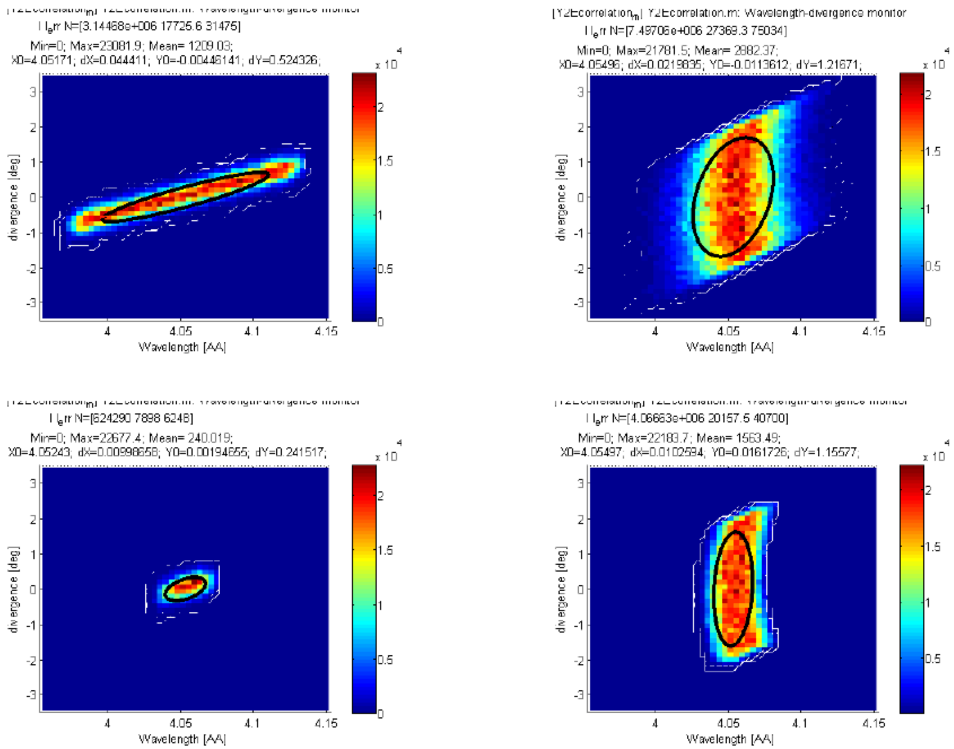
Checks of M.C.: virtual source-monochromator

- McStas simulations versus the analytical Popovici model
- ($\Delta\lambda_i$,γ_1) phase space element, virtual source width = 1 cm

flat | focused

10 cm sample width

2 cm sample width



- horizontal focusing effects:
  → increases beam monochromaticity (10 cm sample)
  → larger divergence (Liouville's theorem)

- no pronounced structures in the intensity landscapes

- resolution ellipses from the gaussian Popovici approximation agree well (lines of 50% probability)

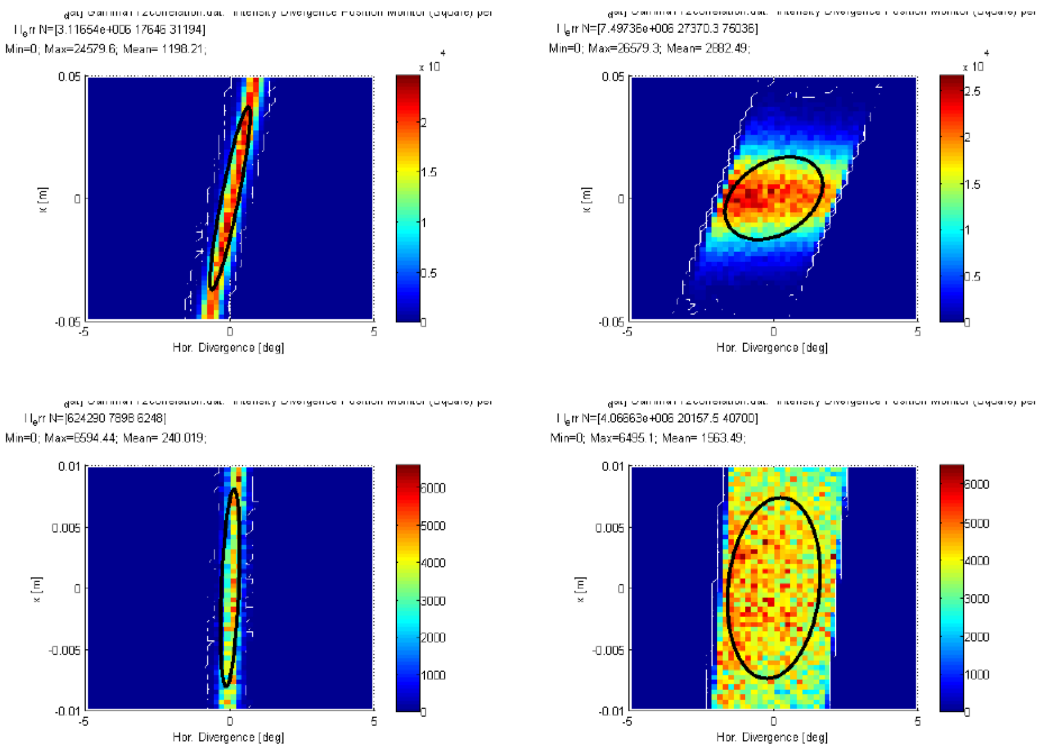
Checks of M.C.: virtual source-monochromator

- McStas simulations versus the analytical Popovici model
- $(\Delta y_2, \gamma_1)$ phase space element, virtual source width = 1 cm

flat | focused

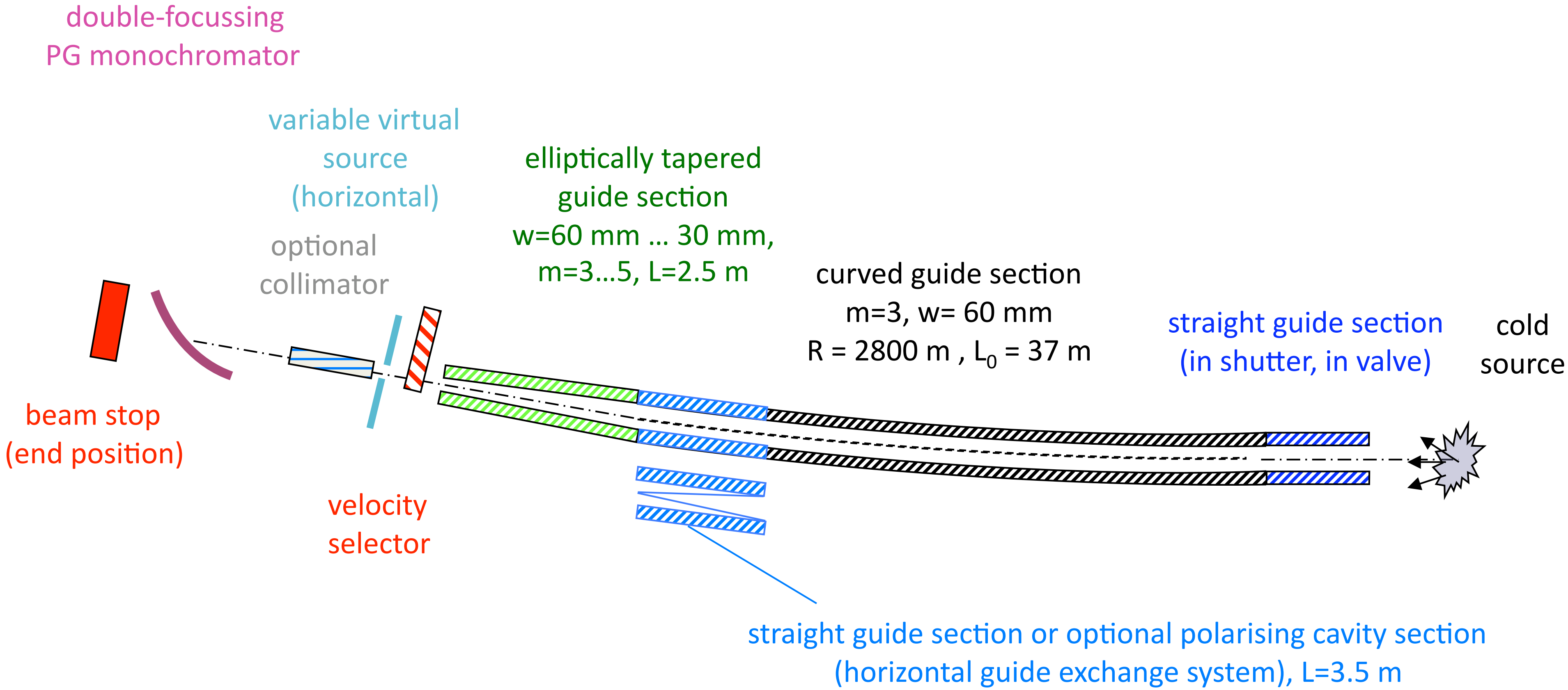
10 cm sample width

2 cm sample width

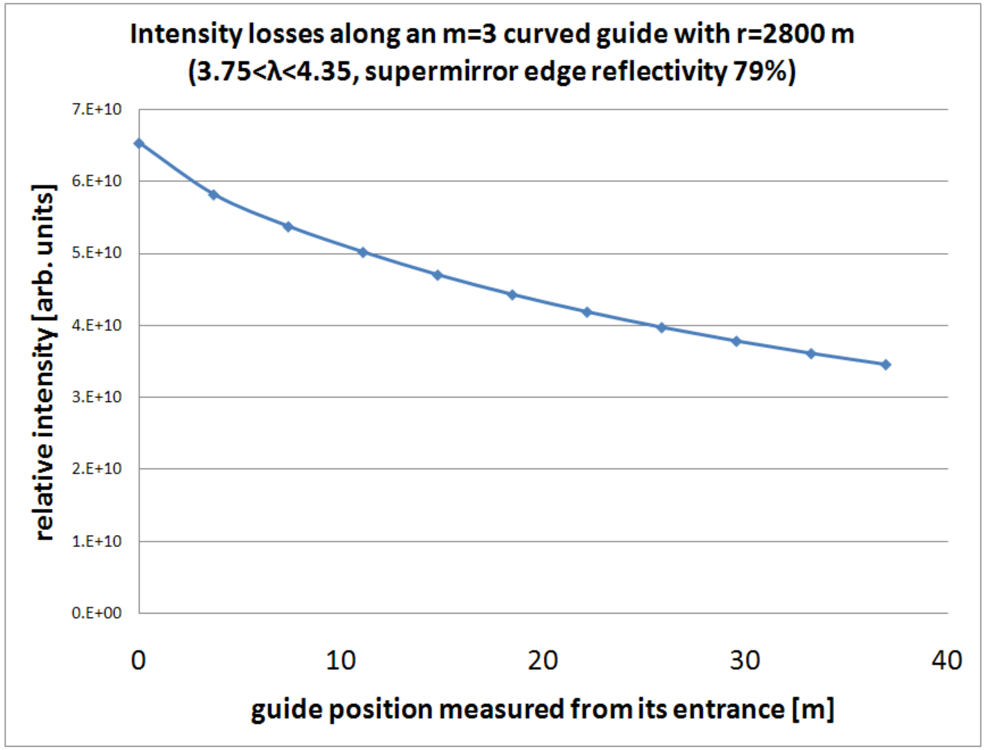


- horizontal focusing effects:
  → spatial focusing
  → increased divergence
  (Liouville's theorem)
- no pronounced structures in the intensity landscapes
- see some deviations but overall good agreement with the gaussian Popovici approximation (lines of 50% probability)

Curved guide simulations



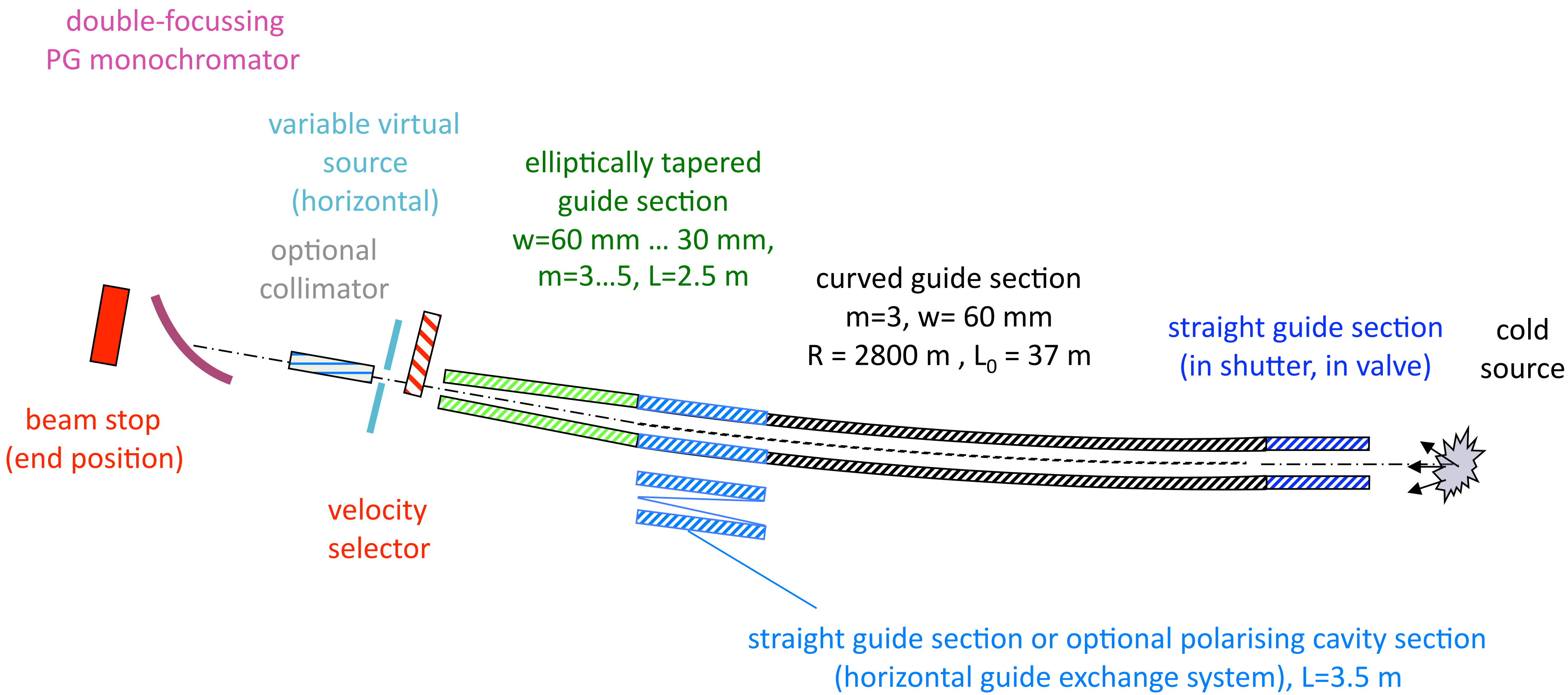
Curved guide simulations



- about 53% of the neutrons survive down the NL1b guide
- vertical and horizontal beam divergences at the end of the guide drop to 70% from their initial values at the guide entrance (in agreement with intensity losses)
- $m_{effective}$=2.1 at the end of the guide
- analytical cut-off wavelength λ*=1.26 Å for m=3 and 1.89 Å for m=2 (compared to 2.2 Å in current FLEX)

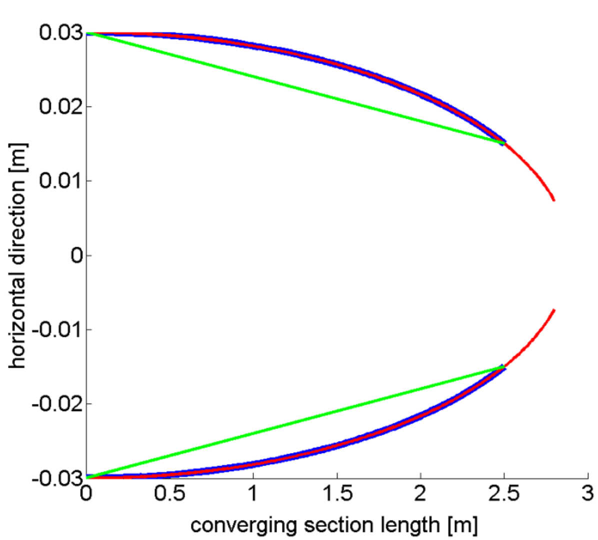
- the guide m coating and entrance position match almost perfectly with the beam that is delivered at that point (from "perfect" m=3 simulations)
- can extend our spectrum towards thermal range

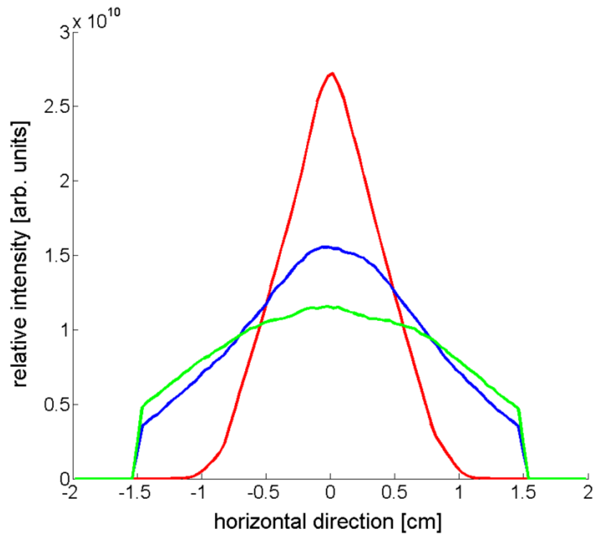
Elliptical section simulations



Elliptical section simulations

• Vitess results at the **virtual source position** for various converging sections

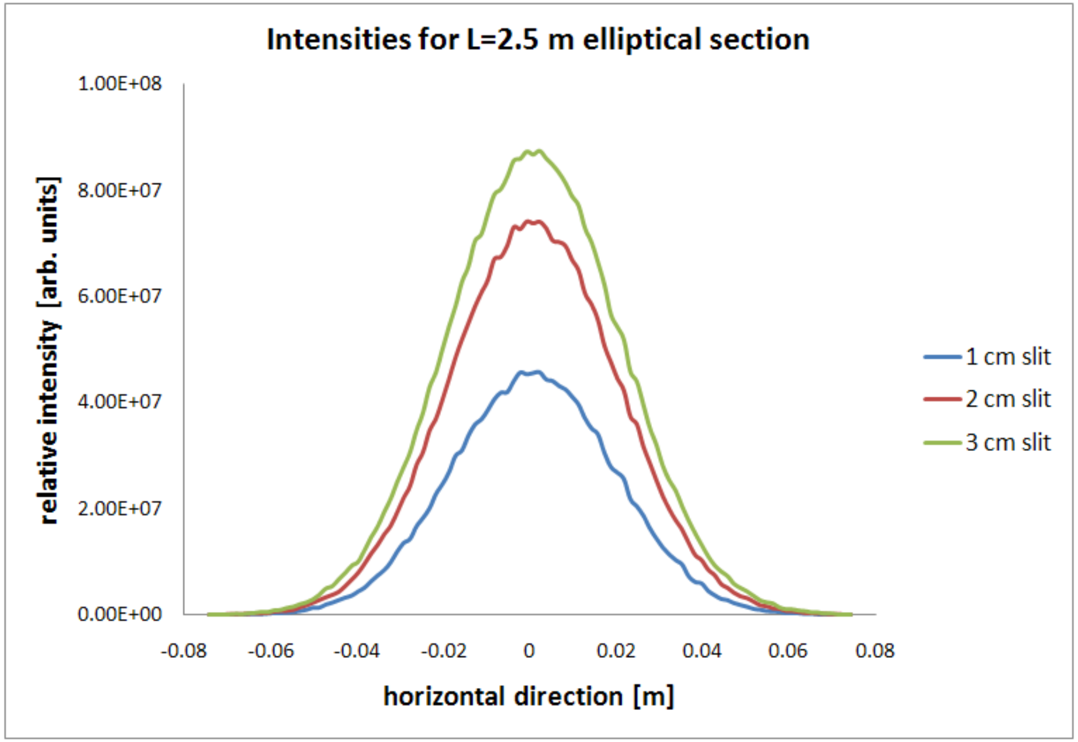




• neutrons are focused according to ray optics, at the ellipse's focal point (no wavelength dependence)
• for small slit sizes the extended ellipse offers large intensity gains at virtual source (and sample) position at the expense of increased beam divergence
• expect this since it spatially focuses more
• for vertical focusing it is better to use the monochromator, since an elliptical shape in this direction will only transport half of the neutron flux

Elliptical section simulations

• Vitess-McStas results at the **sample position** for the 2.5m long converging section



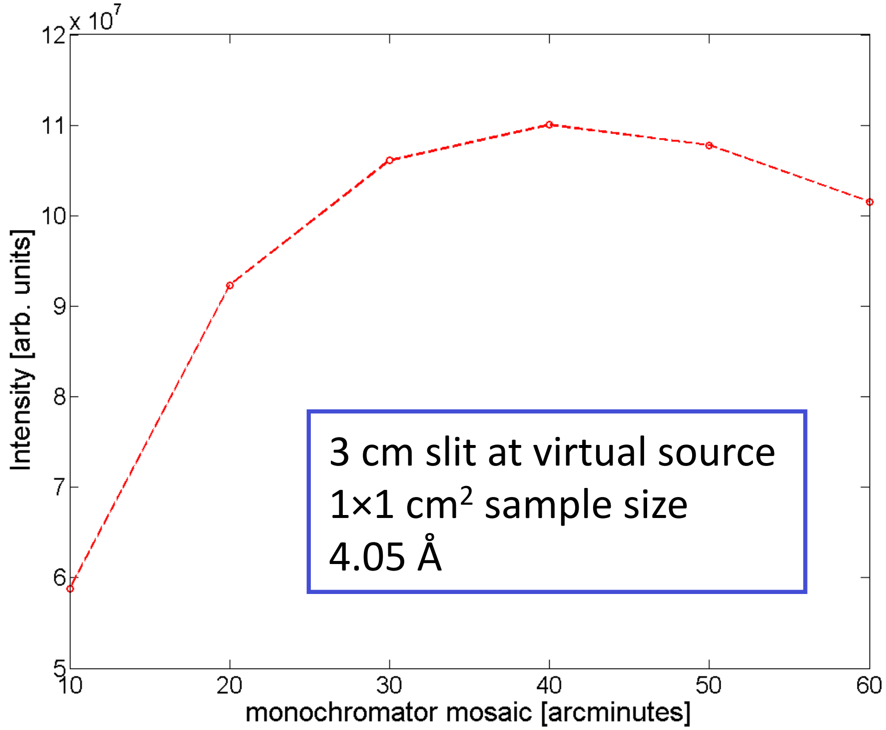
• intensity gains for bigger slit sizes at virtual source are accompanied by losses in energy resolution
• in this case the FWHM of 1×1cm^2 energy monitors are 43, 57 and 70 µeV
• beam divergence is unaffected by slit size...
• ...but depends on converging section shape (the more you try to focus, the higher the divergence)

• we need the truly elliptical shape, otherwise divergence at sample position has a structure
• ΔE at sample position can be tailored for a particular experiment by changing slit size
• a slit at a PSD is equivalent to the slit at virtual source, hence experimentalist can select whether he needs more flux or better ΔE after the experiment, by masking the detector

Monochromator simulations

PG (002) monochromator tested with various virtual source slit and sample sizes

Mosaic spread optimization

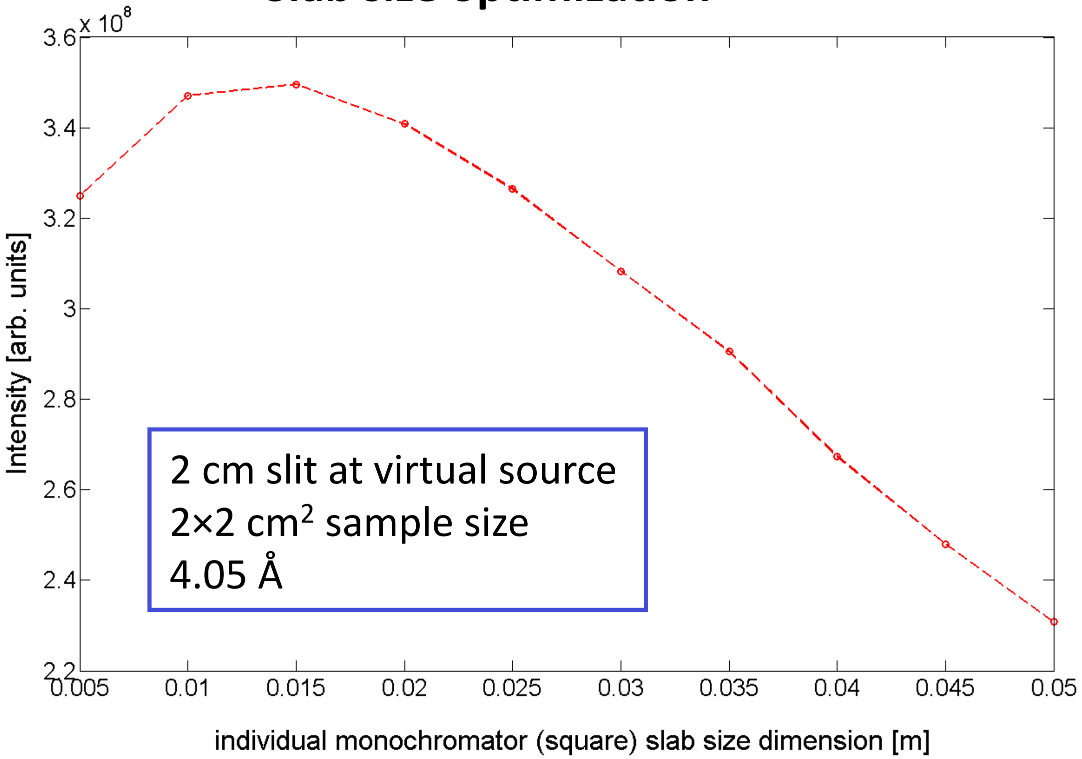


- the integrated intensity of monitors at sample position have a maximum (or plateau) at around 40 arcminutes
- beam is relatively uniform over a 3×3 cm^2 area
- upon reducing slit size, energy resolution gets better at the expense of neutron flux
- horizontal divergence stays relatively unaffected, because the horizontal radius of curvature dominates in divergence

Monochromator simulations

PG (002) monochromator tested with various virtual source slit and sample sizes

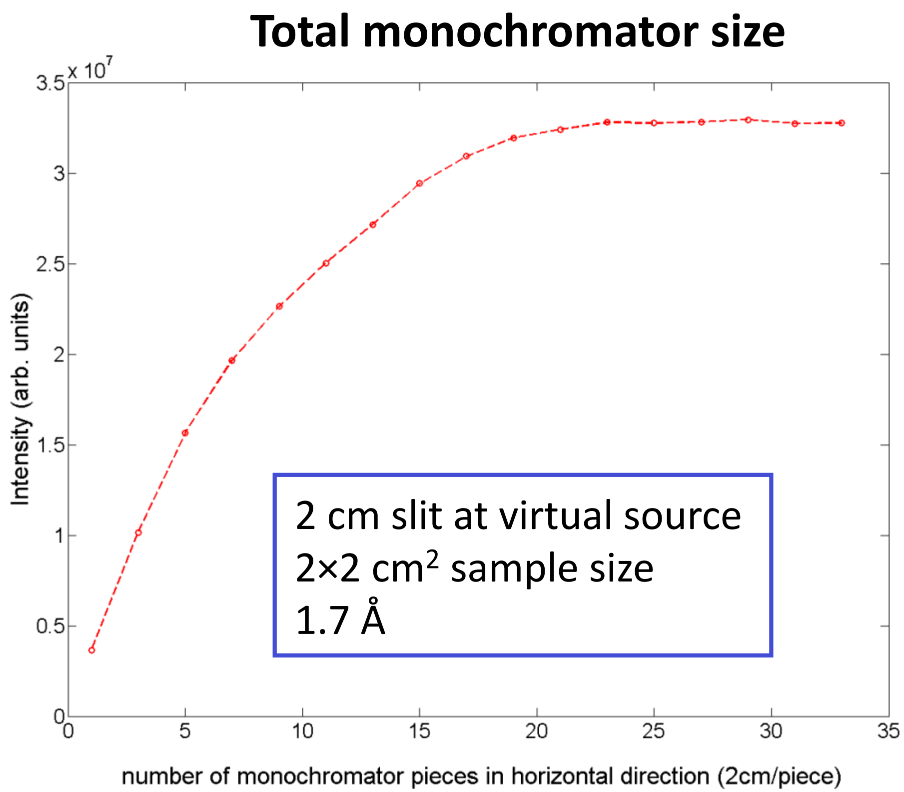
Slab size optimization



- a 1.5×1.5 cm^2 slab gives the highest flux
- a 0.5 mm gap has been assumed in between all slabs
- losses at low slab sizes are due to this gap
- energy resolution is unaffected by slab size

Monochromator simulations

PG (002) monochromator tested with various virtual source slit and sample sizes



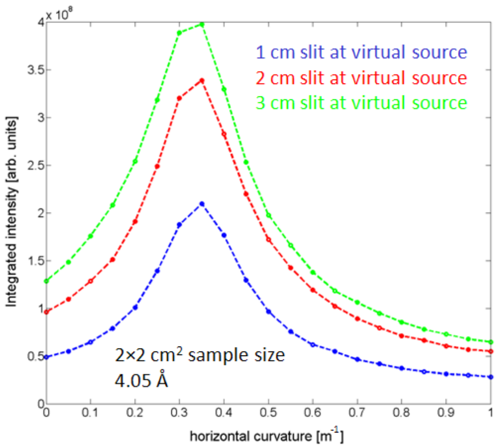
- use shortest FLEX wavelength, 1.7 Å, to get largest monochromator size needed in horizontal direction

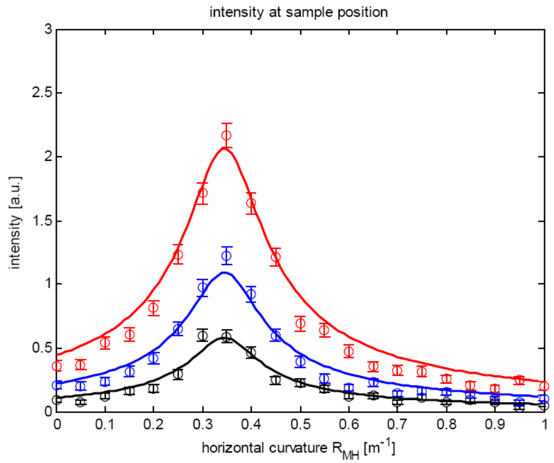
- reach maximum after ≈38 cm

- simple geometrical calculation gives ≈37 cm!

Monochromator simulations

Horizontal focusing effects at sample position





- intensity gains of 3 - 4.5...
- ... at the expense of divergence
- energy spread is unnafected

Maximum possible gain from horizontal focusing (30’ mosaicity)

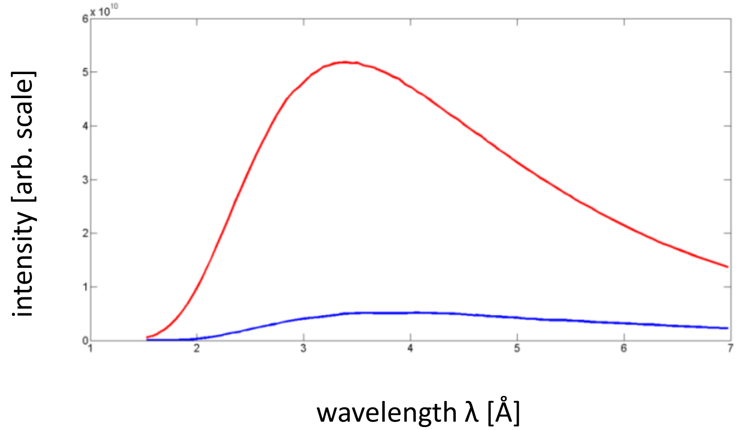
slit size	sample size	simple analytical model	“real” upgraded FLEX guide system
2 cm	2 cm	4.65	4.51
1 cm	2 cm	4.91	5.59
1 cm	1 cm	5.21	6.25

- simulations of complicated FLEX guide system agree well with simple case analytical model
- in the upgrade, we benefit all that is possible from horizontal focusing at sample position!

Overall gain factors for FLEX 2011

Optimized instrument parameters with Vitess and McStas

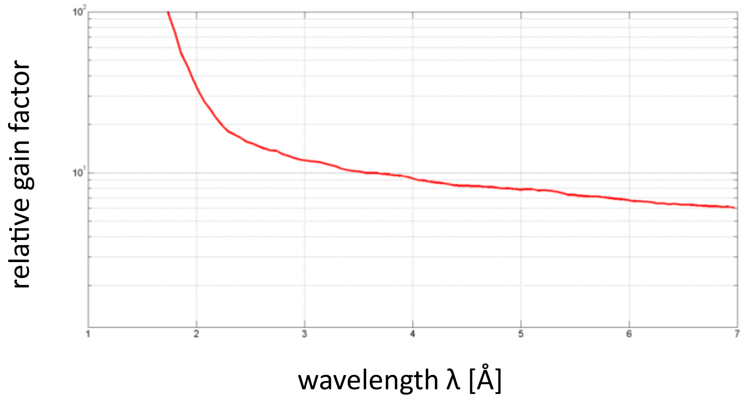
Intensity gains at the end of the guide system



Intensity gains at the sample position
(excluding gains from cold source)

wavelength λ [Å]	intensity gain at sample position	gain in energy resolution	total gain factor
2.36	12.9	1.08	13.9
4.05	6.8	1.34	9.1
6.6	5.5	1.72	9.5

Relative intensity gain for the guide system



- **order of magnitude gain factors**
- **extended thermal neutron range**
- **enhanced polarized neutron flux**

Conclusions – future outlook

- thanks to Vitess and McStas Monte Carlo codes we have a good description of the primary spectrometer
- virtual source – horizontal monochromator focusing will match horizontal to vertical Q resolution
- energy resolution can be tailored by slit size (and collimators)
- big intensity gains, increased energy resolution and extended energy transfer from 8 to 20 meV, towards thermal range
- prefer Vitess for the guide system (especially elliptical section)
- McStas has been extensively tested and works perfect in the infinitely thin crystal limit approximation

- need a secondary spectrometer description
- polarized section simulations