# Towards virtual experiments: How well can we simulate existing instruments?

- HET – Update
- IN16 and IN14 at the beam line H53 at ILL
- Optimizing the beam line H112 at ILL

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# Towards virtual experiments: How well can we simulate existing instruments?

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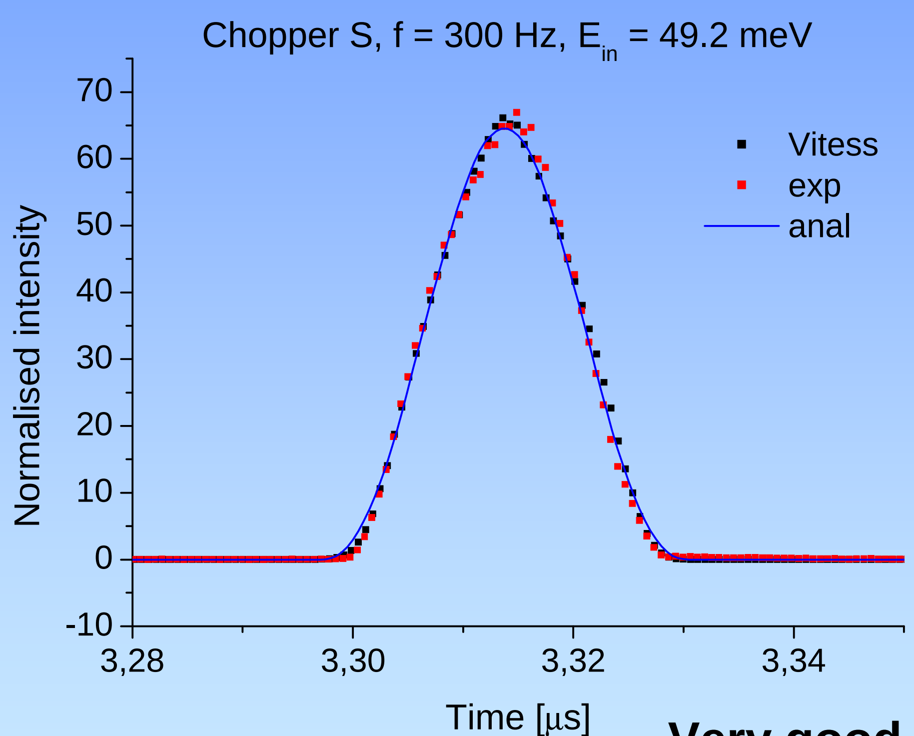
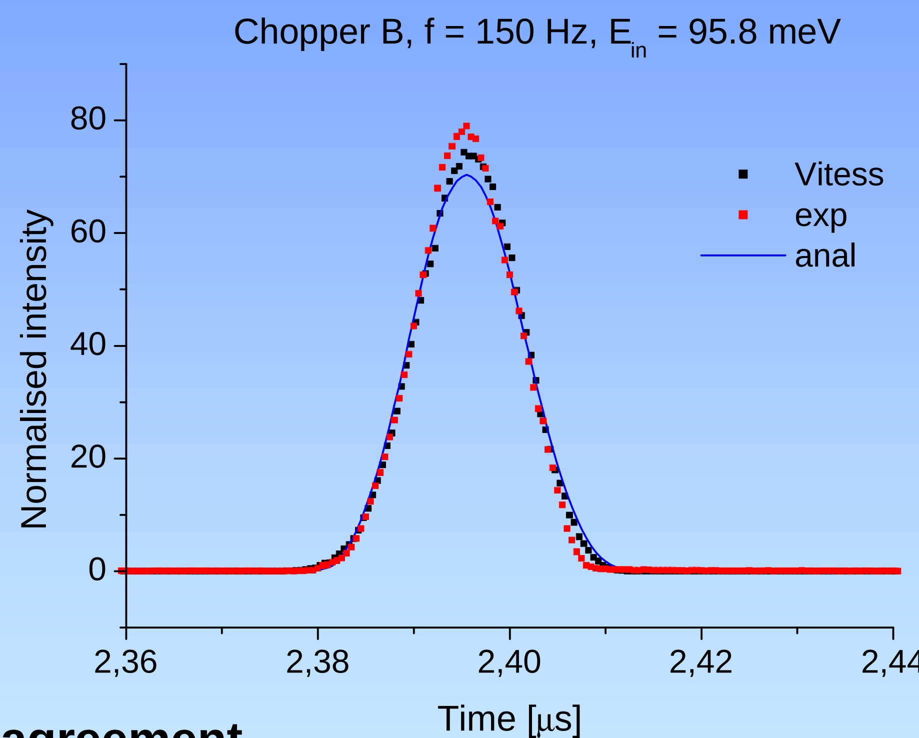
# Using Fermi choppers to shape the neutron pulse

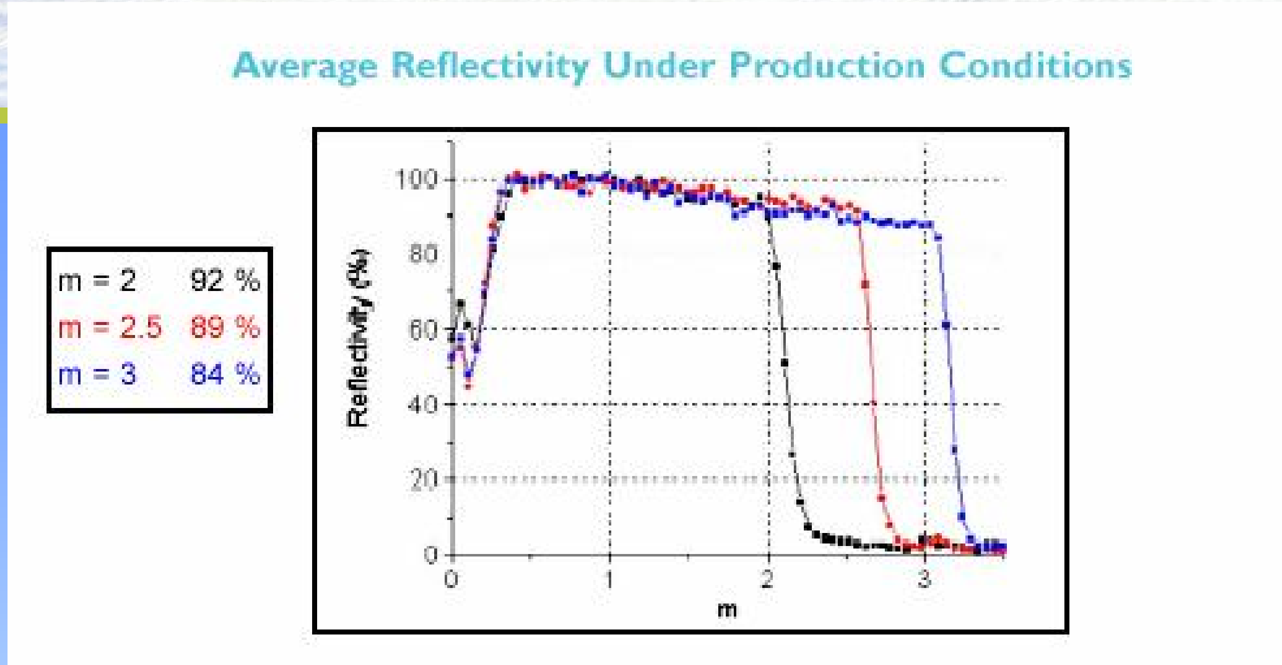
***Better moderator description using MCNP***
***Improvement on the VITESS FC module***
***Correct geometrical description of the FC packages B and S***




**Very good agreement**


J. Peters, J.D.M. Champion, G. Zsigmond, H. N. Bordallo, F. Mezei to be submitted to NIMA
J. Peters, Nucl. Instr. Meth. Phys. Res. **A540** (2005), 419 - 429.
H.N. Bordallo, G. Zsigmond and J. D. M. Champion, Physica **B350** (2004), e717 – e719.



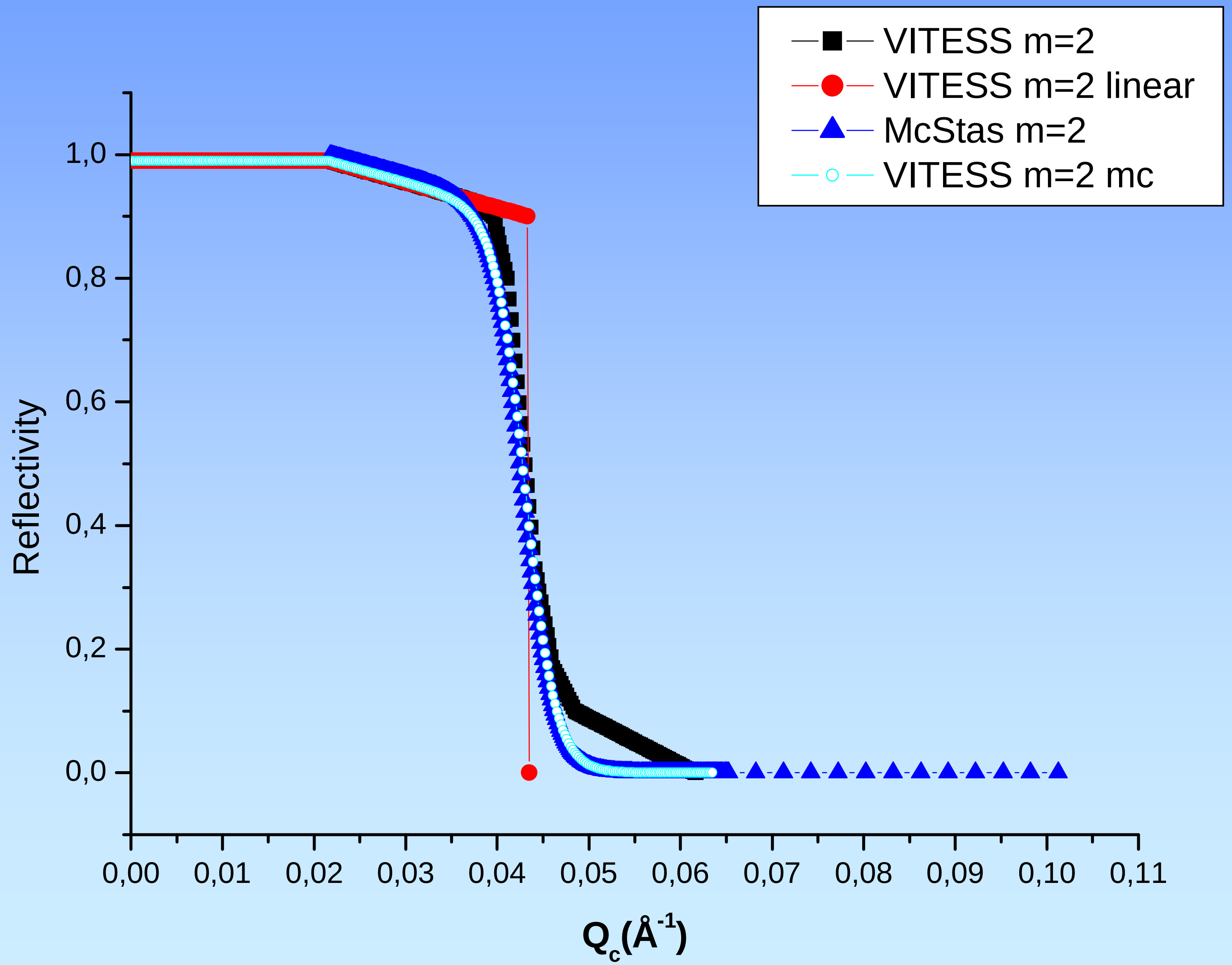

Taken from
http://www.lesker.com/newweb/Downloads/pdf/mirrortron.pdf

$$R = \begin{cases} 1 & Q < Q_c \\ \frac{1}{2}\left(1 - \alpha(Q - Q_c)\right) & Q > Q_c \end{cases}$$

$$(1 - \alpha Q_c) = R$$

**for example, if α = 4.5 R = 0.9**

# Equal SM descriptions in McStas and VITESS



# The intensity distribution in a long curved guide as function of l

- Idea: how accurate is the description of a curved guide?
- Action: check the Maier-Leibnitz guide formula
- Result: guide description seems to be ok

# The critical parameters of a long curved guide

$\gamma^* = (2a/\rho)^{1/2}$; $\gamma^*$ = characteristic angle;

With $\gamma^* = k_\perp / k^*$ we get: $k^* = k_\perp (2a/\rho)^{-1/2}$; $k^*$ = characteristic k-vector;

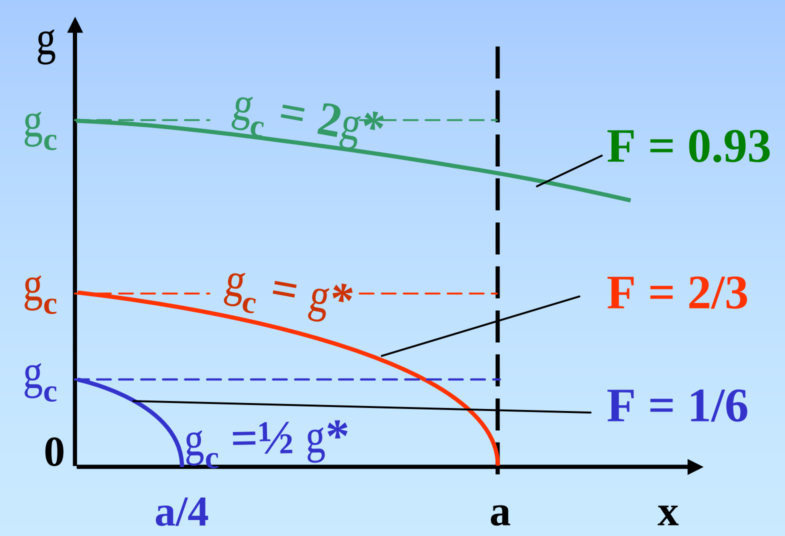
With $\lambda^* = 2\pi / k^*$ we get: $\lambda^* = 2\pi (2a/\rho)^{1/2} / k_\perp$; $\lambda^*$ = characteristic wavelength;

**Filling factor F** (intensity ratio curved guide/straight guide): $F\left[\gamma = (\gamma_c^{\,2} - 2x/\rho)^{1/2} / \gamma = \gamma_c\right]$

$$F = \frac{1}{a\gamma_c}\int_0^{a^*} dx\,\gamma = \frac{1}{a}\int_0^{a^*} dx\left(1 - \frac{2x}{\rho\cdot\gamma_c^2}\right)^{1/2}$$

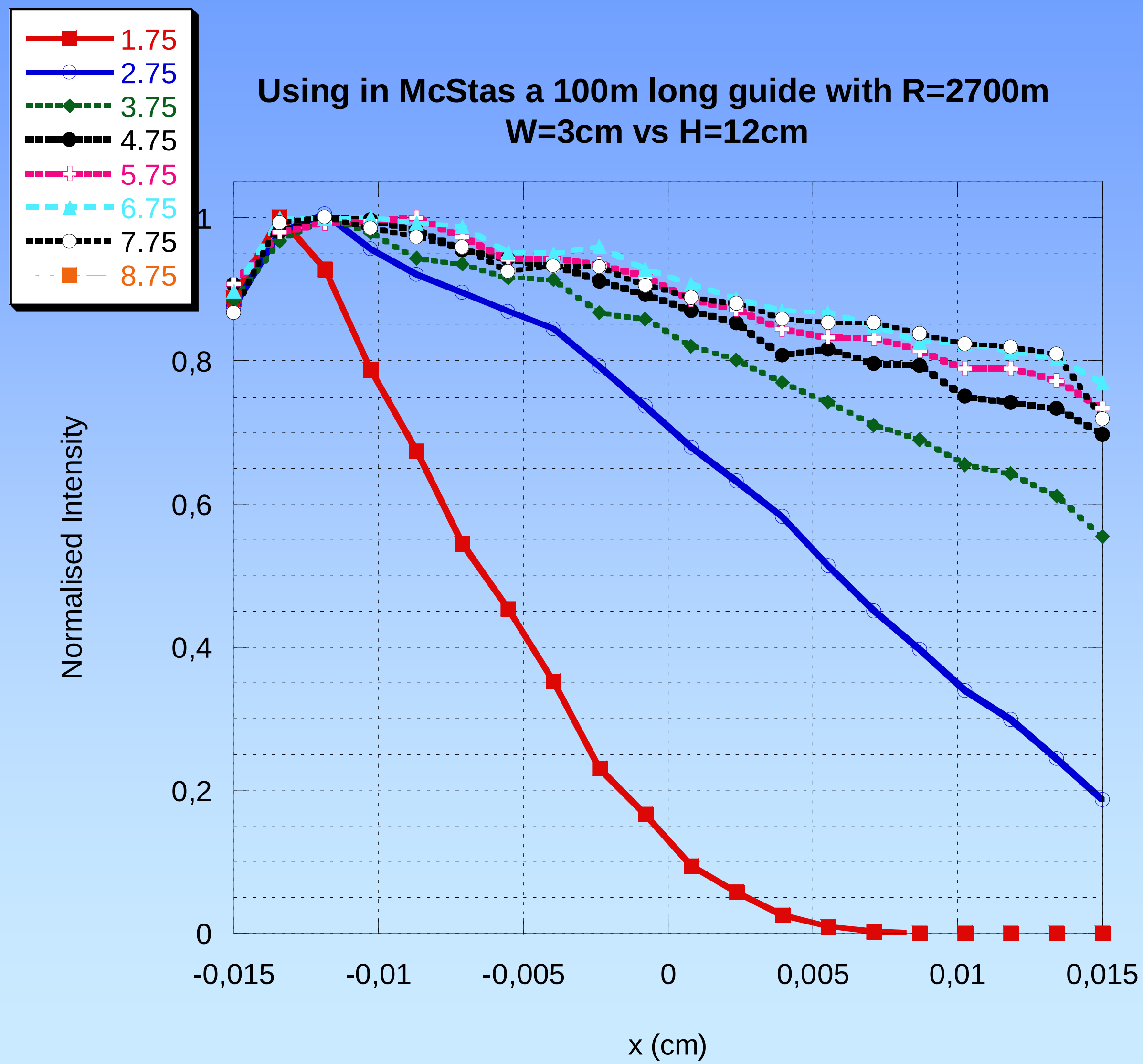
$a^* = a$ for $\gamma_c \geq \gamma^*$;

$a^* = \rho\,\gamma_c^{\,2}/2$ for $\gamma_c \leq \gamma^*$;



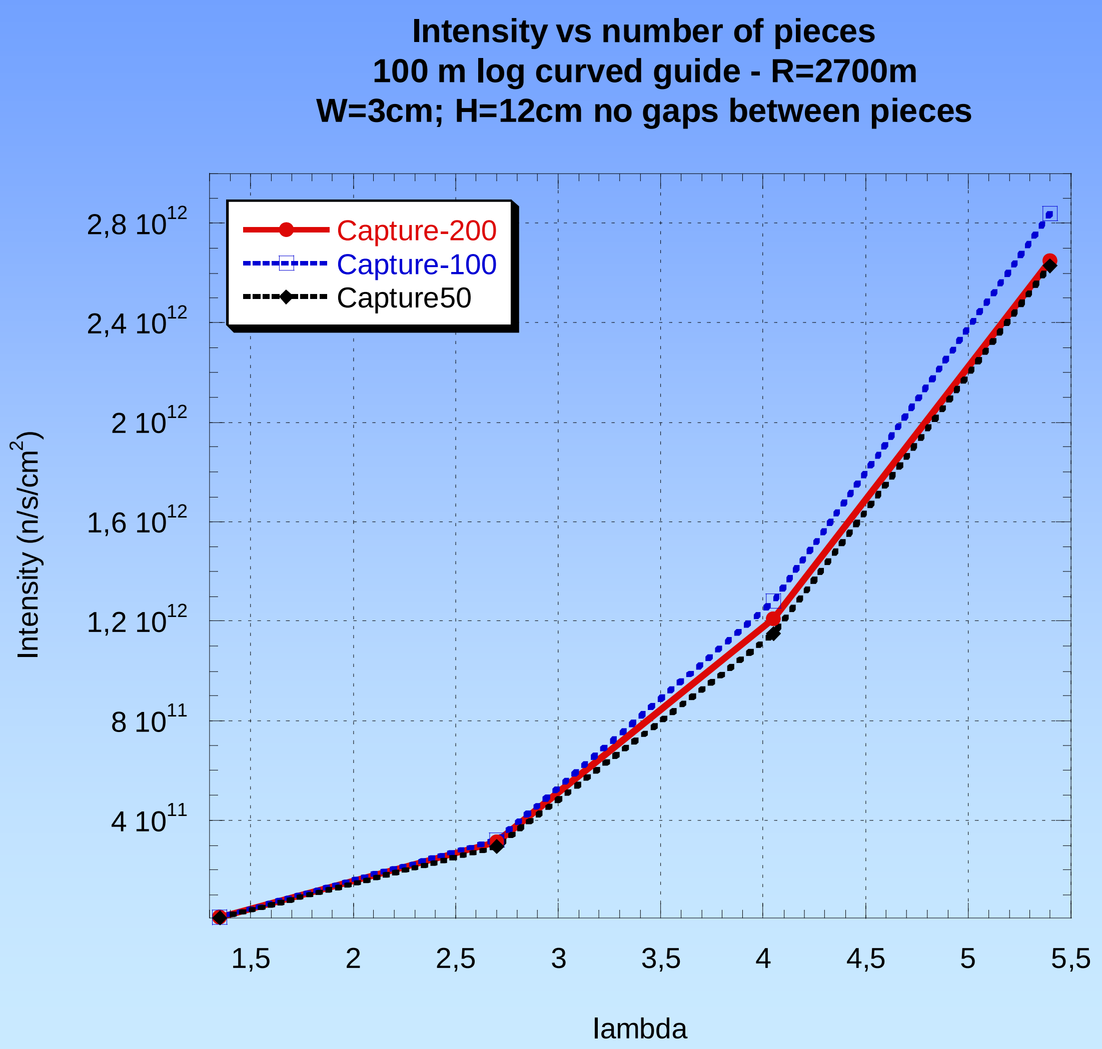

$F(\gamma_c = \gamma^*) = 2/3$; $F(\gamma_c = 2\gamma^*) = 0.93$; $F(\gamma_c = \gamma^*/2) = 1/6$;

Simulations were performed for a 100m long curved guide, divided in 50,100 and 200 pieces with R = ρ = 2700 m, width x = 0.03m and height = 0.12 m, giving a critical wavelength, $\lambda c = 2.7$Å.



- A 100 m long curved guide made of 100x1m pieces without gaps in between the pieces seems to be the optimized design.

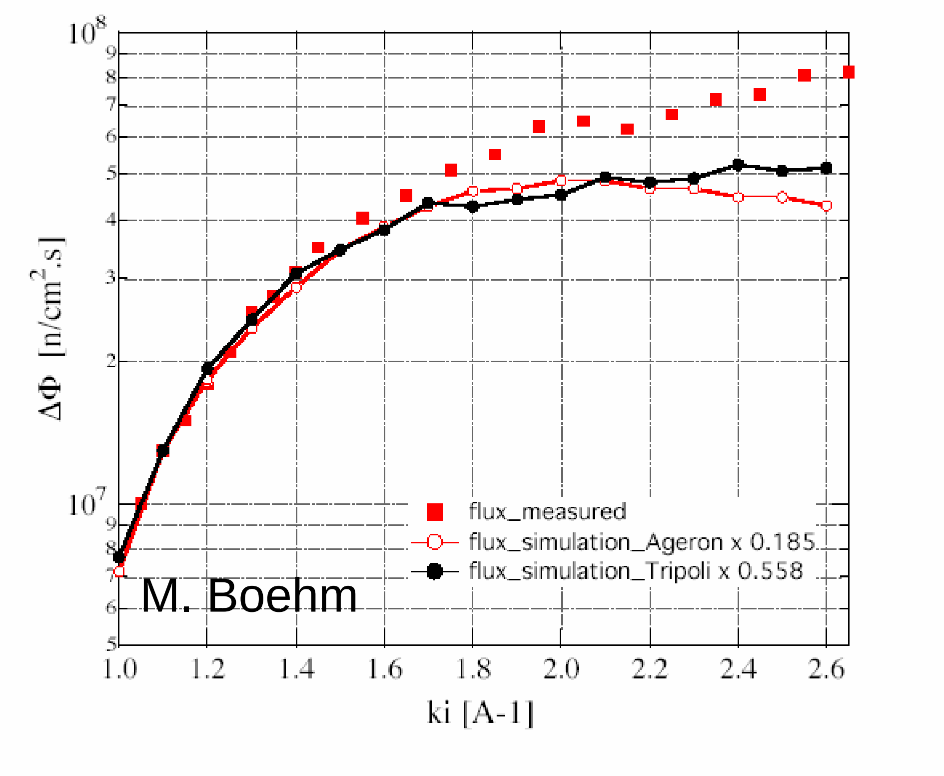
- The increase of gaps can decrease the intensity. Over 100 m a total gap of 2m can cause a loss of at least 5% in the total flux.

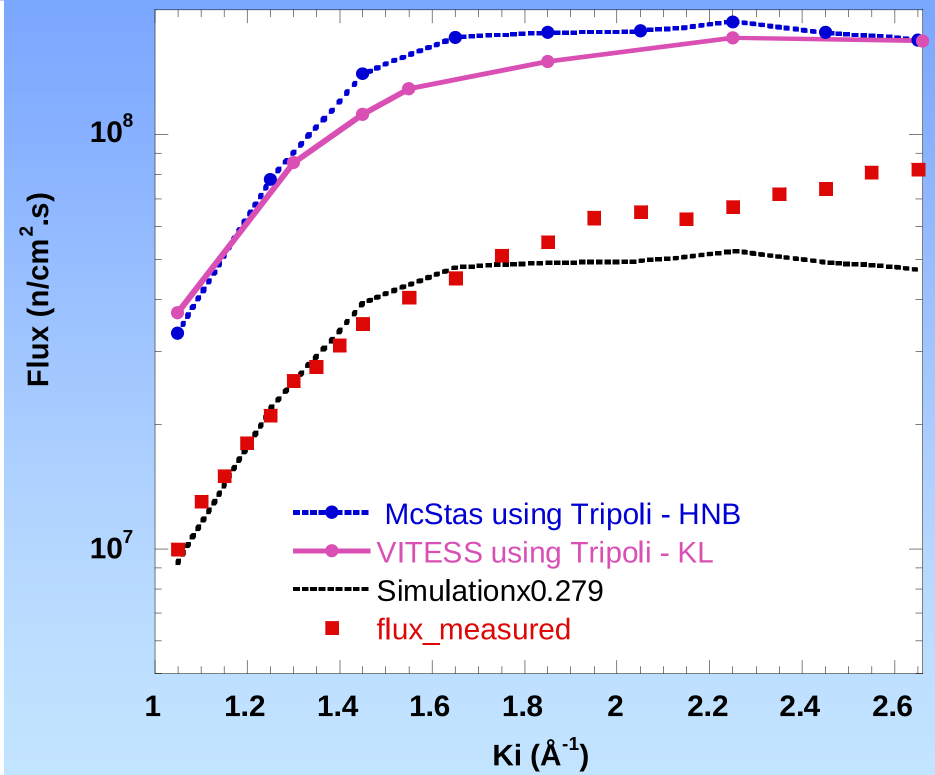


# The beam line H53 at ILL

- Goal 1: benchmark the backscattering IN16
- Goal 2: simulate the new IN16b and decide the best position and guide design
- Need 1: accurate capture flux as well as monochromatic flux
- Need 2 : accurate description of the divergence

# IN14: Check the source description




**Tripoli calculations: G. Campioni, Thèse de 3eme cycle universitaire, CEA-Saclay-France 2004**

# H53 – Preliminary results

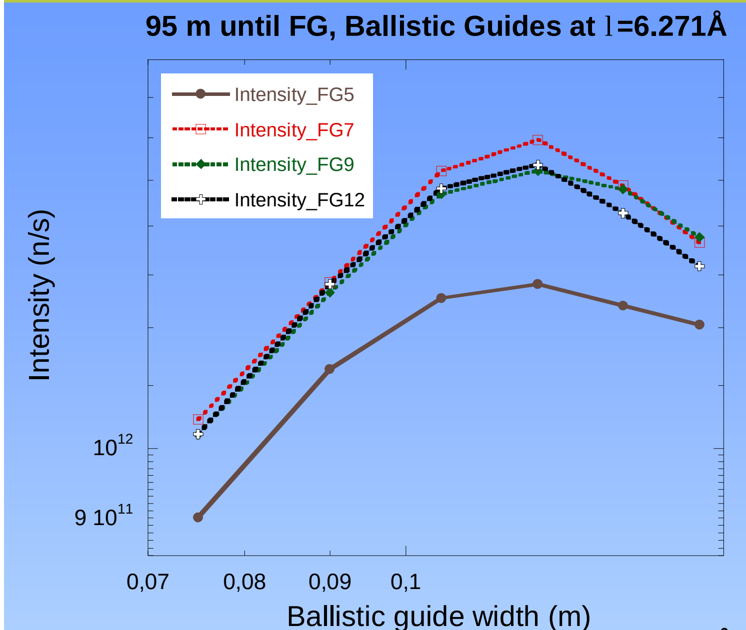
- With Tripoli we can estimate quite well the capture flux
- The evolution of the shape of monochromatic wavelength can be described; the intensity is too high

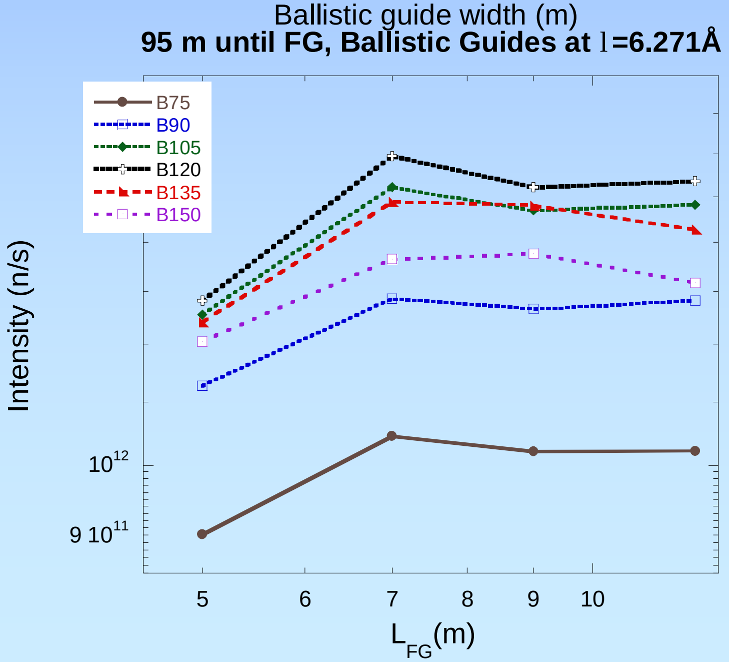
# The beam line H112 at ILL

- Goal 1: optimization of the guide design
- Goal 2: simulate the new IN16b based on various possibilities for the guide layout
- Need 1: accurate capture flux as well as monochromatic flux
- Need 2 : accurate description of the divergence

| Position (m) | McStas_curvedguide<br>Intensity (n/s)<br>Source_gen:VCS | McStas_guide<br>Intensity (n/s)<br>Source_gen:VCS | VITESS_window<br>Intensity (n/s)<br>Source_gen:VCS |
|---|---|---|---|
| 2.335 | $1.40e^{+12}$ | $1.40e^{+12}$ | $1.37e^{+12}$ |
| 5.505 (6.6x12cm2) | $4.16e^{+11}$ | $4.16e^{+11}$ | $3.87e^{+11}$ |
| 5.826<br>(6.0x12cm2)<br>converging | $3.94e^{+11}$ | 3.94e+11 | $3.76e^{+11}$ |
| 11.905<br>diverging | $3.03e^{+11}$ | 3.03e+11 | $3.06e^{+11}$ |
| 20.366<br>curved | $2.81e^{+11}$ | 2.36e+11 | $2.85e^{+11}$ |
| 28.340<br>curved | $2.63e^{+11}$ | 2.19e+11 | $2.71e^{+11}$ |
| 31.227<br>curved | $2.51e^{+11}$ | 2.09e+11 | $2.64e^{+11}$ |
| 91.227<br>(9x12 cm2) | $1.92e^{+11}$ | 1.65e+11 | $2.07e^{+11}$ |
| Flux n/s.cm$^2$ for 6Å<br>(5-7Å) | $1.78e^{+9}$ | 1.53e+9 | $1.91e^{+10}$ |
| 98.227 (2.5x2.5cm2) | $6.05e^{+10}$ | $5.92^{+10}$ | $6.89^{+10}$ |
| Flux n/s.cm2 for 6Å<br>(5-7Å) | $9.67^{+9}$ | $9.47^{+9}$ | $1.1\ e^{+10}$ |

# Performance of ballistic guides




Guide entrance : 6.6x12cm$^2$

L' ~3m

Guide exit: 6x12cm

Guide diverging part: 6x12 cm$^2$

$L_1$=Opens over 12 m to 9 cm

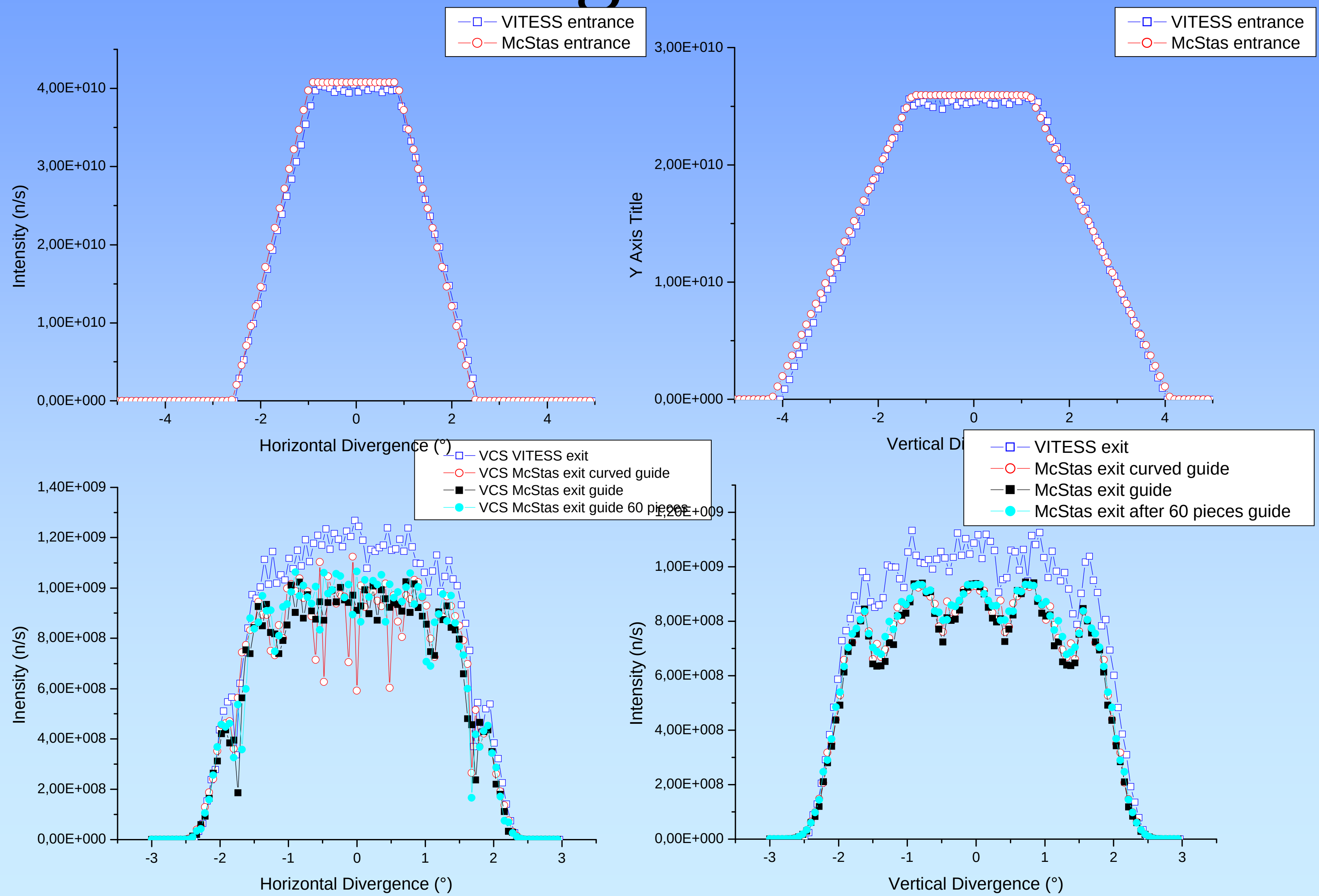
Varies if we want to open more

Focus guide exit: 2.5x2.5cm$^2$

$L_{total}$=100 m

Procedure of optimazation: K.H. Anderson

# H112 – divergence for λ=6Å



# H112 – Preliminary results

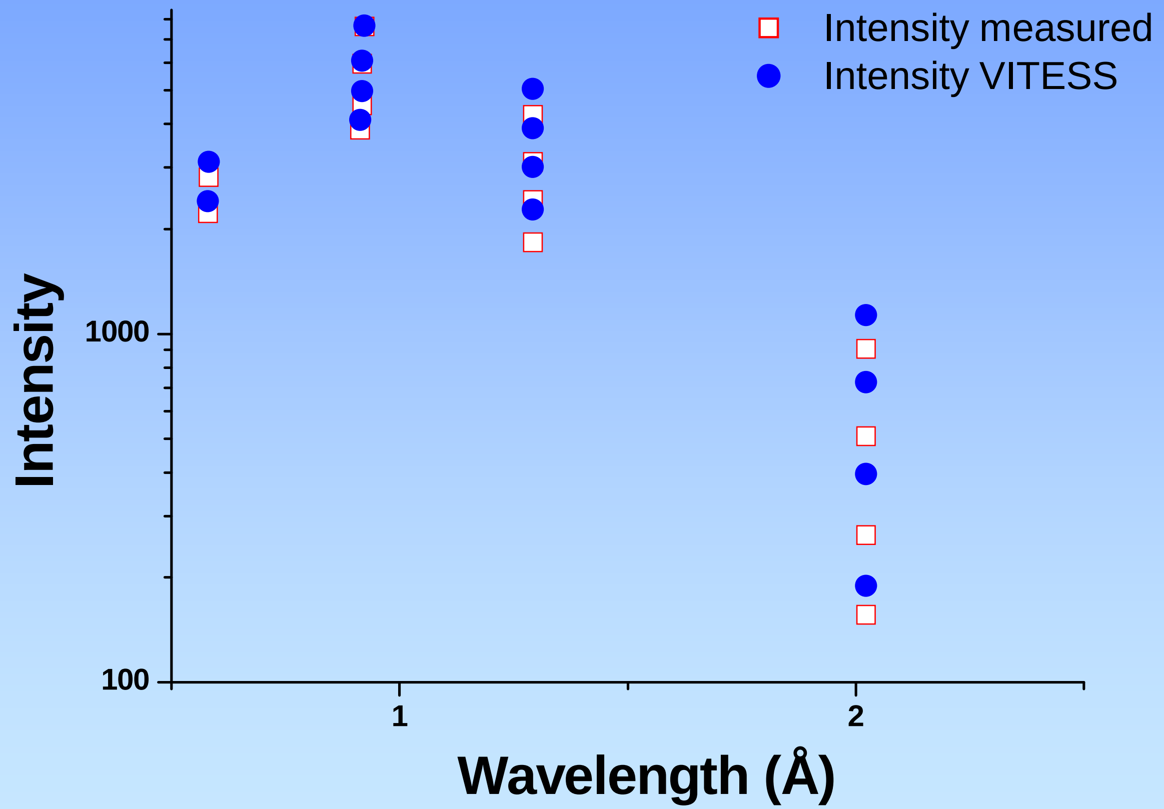
- With an optimized ballistic guide a flux improvement of about 60% can be obtained. Initial calculations by Tilo Seydel using an elliptical guide seems to show that the performance of the instrument could be improved.
- Angular distribution of neutrons exiting the converging guide in the horizontal and vertical directions, is about the same using both packages:

i) for 6Å on gets horizontal divergence ~ 3.5° and vertical divergence about 4°,

ii) for 3Å horizontal divergence = vertical divergence ~ 2°,

- However at some points the profile of the distribution is different. It is very important to understand the origin of such discrepancy.

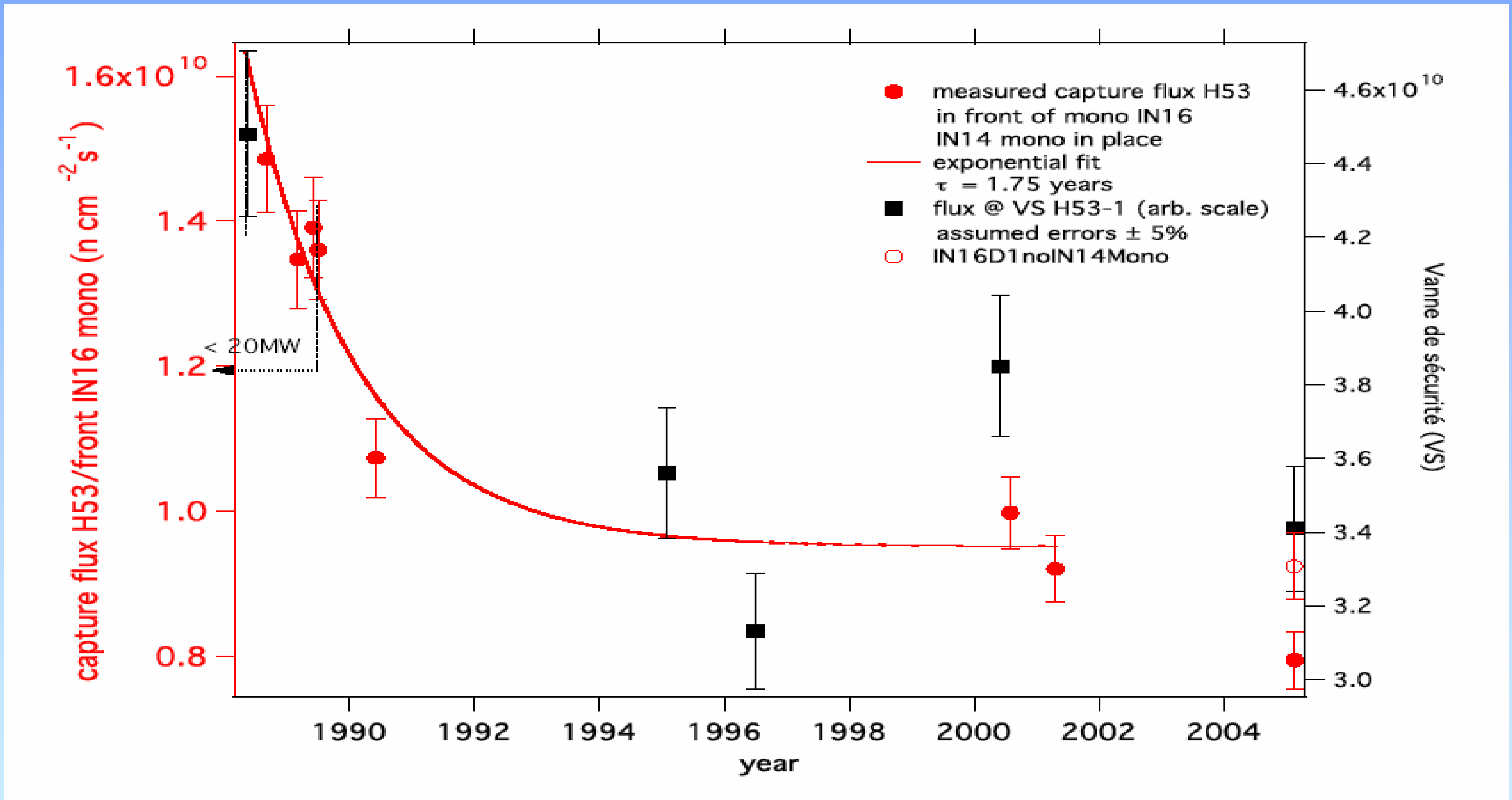
# Question 1




**Integral Intensities: $I_{VITESS}$=factor*$I_{measured}$**

**factor: [0.95,1.5]**

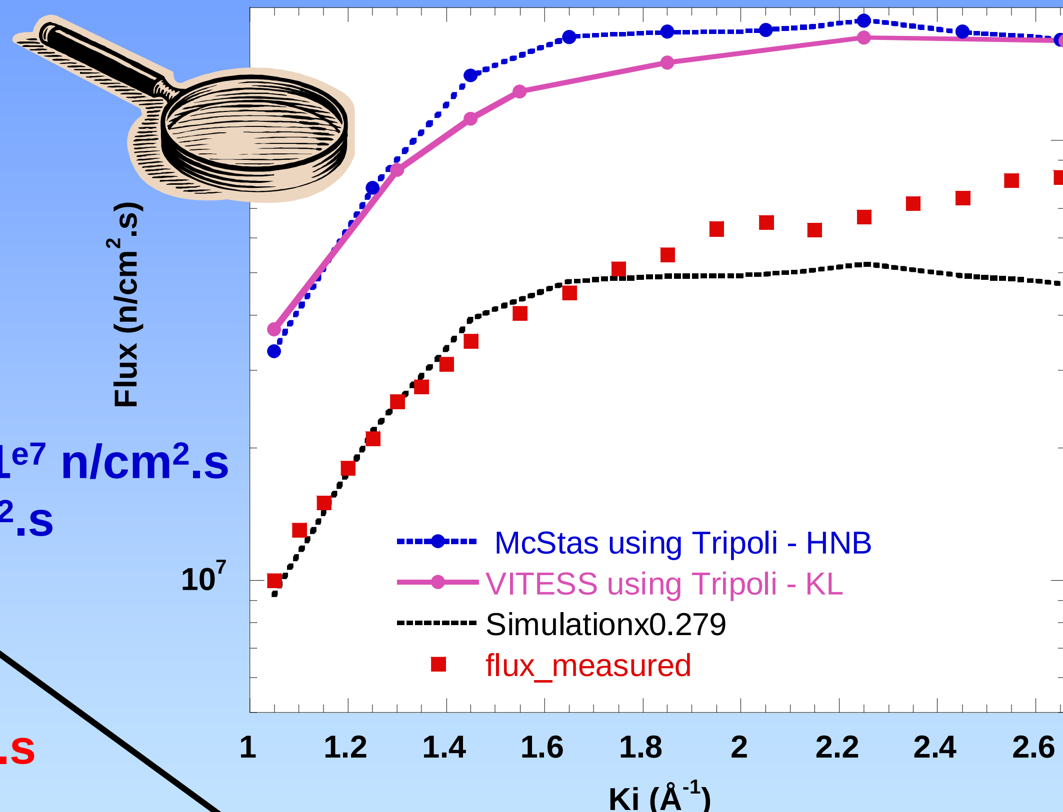
# Question 2




**Questionable accuracy on the gold foil measurements?**

# Question 3

## Should we consider a normalization factor? Why?

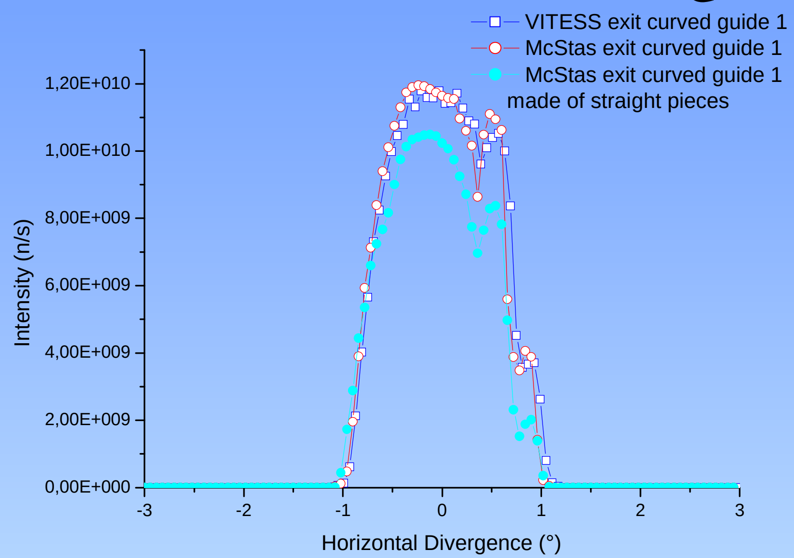



**For $k_i$=1.05Å$^{-1}$ (l~6Å)**
**Flux measured at sample = $1^{e7}$ n/cm$^2$.s**
**Flux simulated ~ 3.5 $e^7$ n/cm$^2$.s**

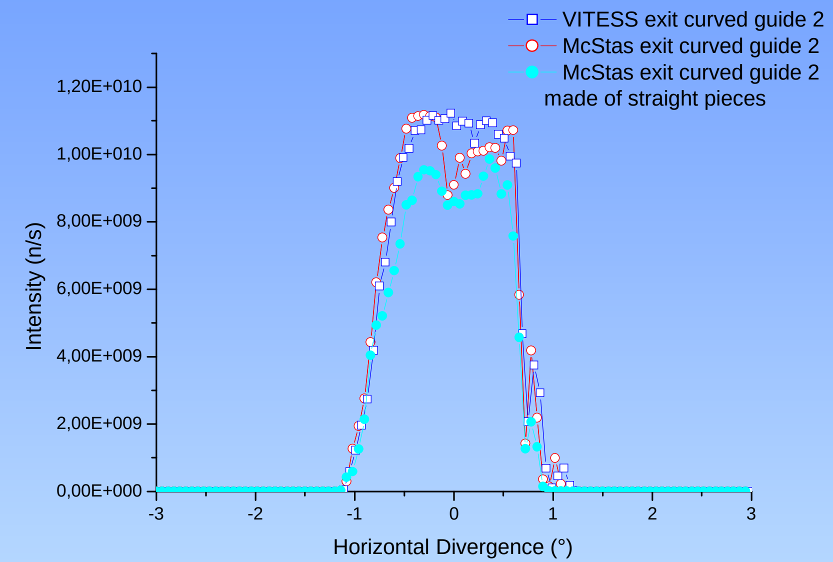
**~$2e^7$ n/cm$^2$.s**

| | | | | |
|---|---|---|---|---|
| IN16 position @ exit FG | ~$1.5e^7$ | $3.14e^8$ | **$2.98e^8$** | No filter, no chopper, no losses due to time |
| IN16 position @exit FG | ~$1.5e^7$ | 7.3 $e^7$ | $7e^7$ | Too high! |

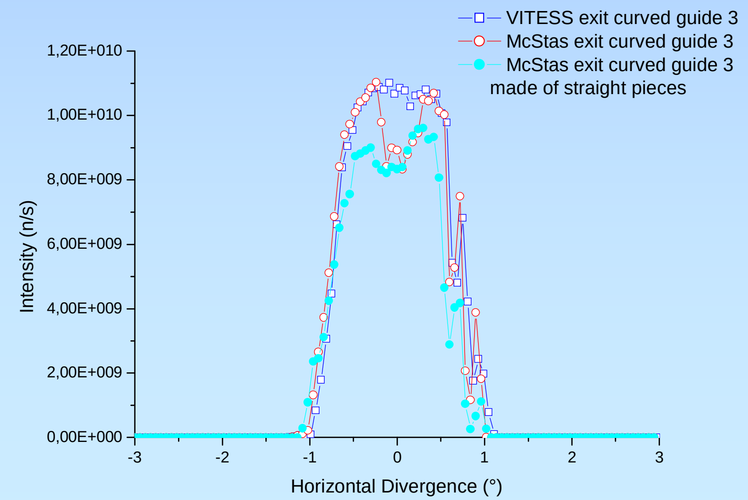
# Question 4



VITESS exit curved guide 1
McStas exit curved guide 1
McStas exit curved guide 1 made of straight pieces
Intensity (n/s)
1,20E+010
1,00E+010
8,00E+009
6,00E+009
4,00E+009
2,00E+009
0,00E+000
-3
-2
-1
0
1
2
3
Horizontal Divergence (°)

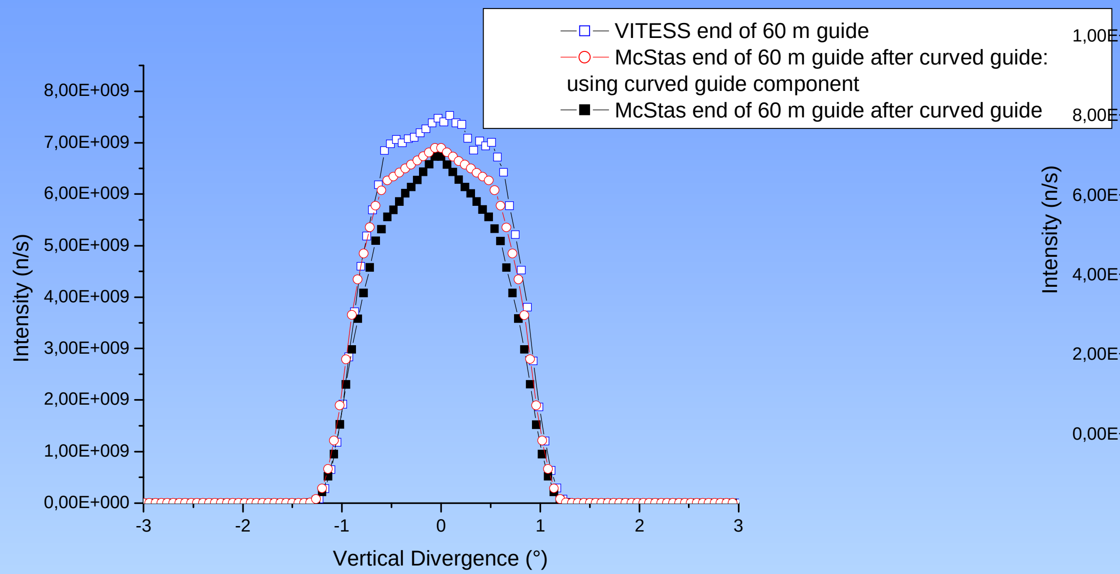



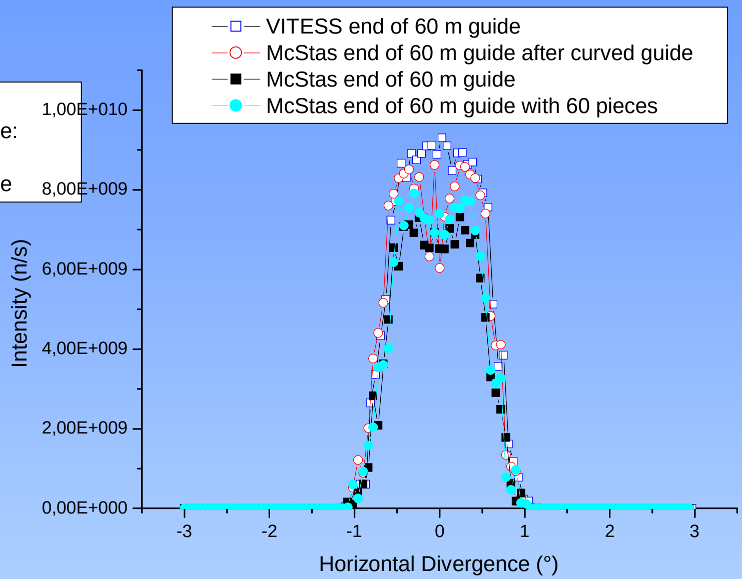
VITESS exit curved guide 2
McStas exit curved guide 2
McStas exit curved guide 2 made of straight pieces
Intensity (n/s)
1,20E+010
1,00E+010
8,00E+009
6,00E+009
4,00E+009
2,00E+009
0,00E+000
-3
-2
-1
0
1
2
3
Horizontal Divergence (°)

VITESS exit curved guide 3
McStas exit curved guide 3
McStas exit curved guide 3 made of straight pieces
Intensity (n/s)
1,20E+010
1,00E+010
8,00E+009
6,00E+009
4,00E+009
2,00E+009
0,00E+000
-3
-2
-1
0
1
2
3
Horizontal Divergence (°)

# Question 4 cont.




# binning effect???

## Face of Tutankhamun reconstructed

The French team created this image of the young king (image: Conseil supérieur des antiquités égyptiennes)

The US team were not told where the skull came from (image: Conseil supérieur des antiquités égyptiennes)

"The results of the three teams were identical or very similar in the basic shape of the face, the size, shape and setting of the eyes, and the proportion of the skull…"
"The primary differences were in the shape of the end of the nose and ears…"
The French and American versions had similar noses and chins, but the Egyptian team gave their reconstruction a stronger nose…

# Acknowledgments


- HET

J. Peters – HMI

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J.D.M. Champion – ISIS

- H53 and H112 guides (simulations, details)

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E. Fahri – ILL

B. Frick - ILL

M. Boehm and A. Wildes–ILL

I. Sutton - ILL

- Guides

K. Anderson

R. Gahler