

**International Workshop on Applications  
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**FOCUS Intercomparison using  
McStas/VITESS/Restrax**

U. Filges<sup>1</sup>, J. Saroun<sup>2</sup>, F. Juranyi<sup>1</sup>, G. Zsigmond<sup>1</sup>

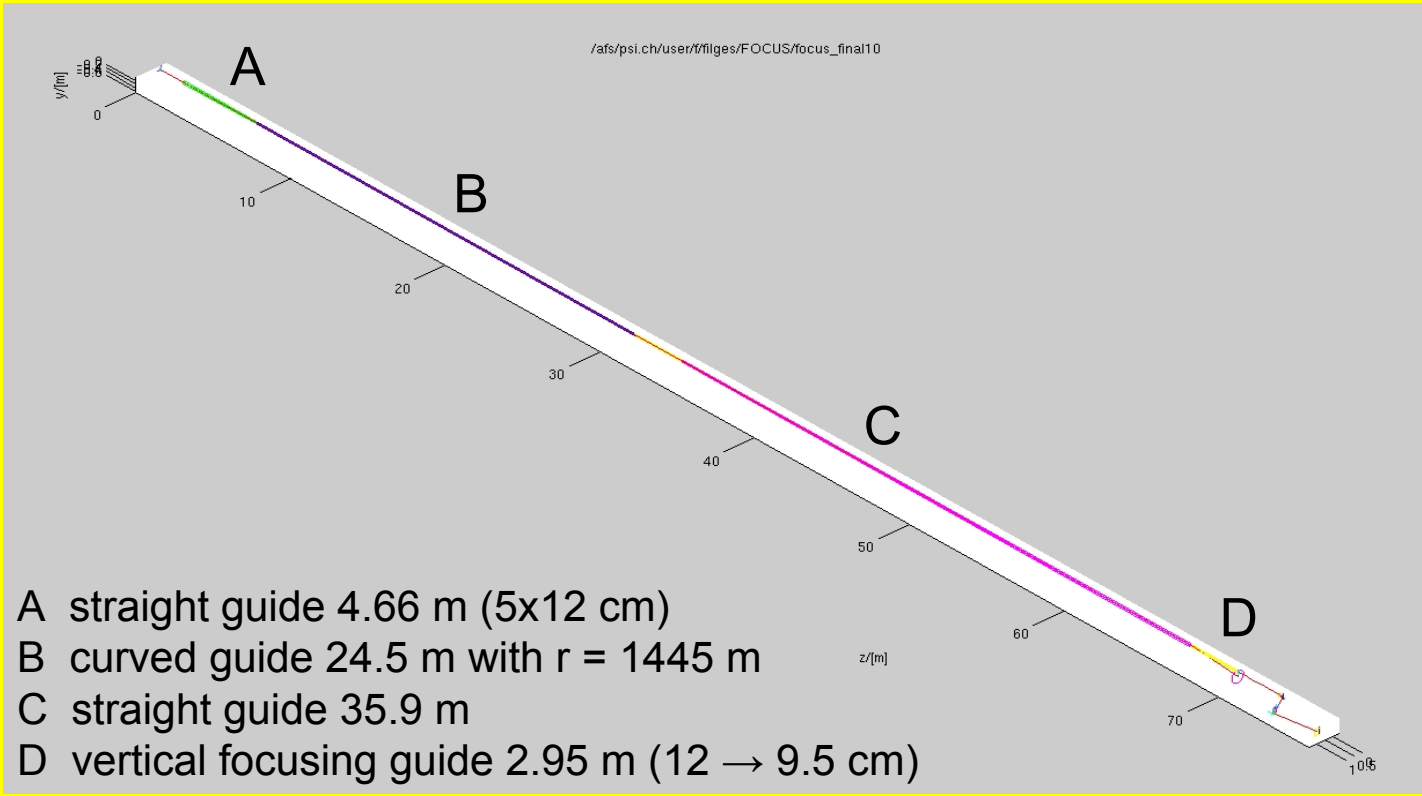
<sup>1</sup>Laboratory for Development and Methods (PSI), Switzerland

<sup>2</sup> Nuclear Physics Institut, Czech Republic

## McStas/VITeSS/Restrax Intercomparison

- package versions
  - McStas 1.8 (Linux)
  - VITeSS 2.6 (Linux)
  - Simres-Restrax 5.0.3 (Linux)
- including a two part intercomparison:
  - the FOCUS guide system and
  - the FOCUS instrument itself
- FOCUS Guide system was completely simulated in the wavelength range of 0.1 – 20 Å using both flat and Maxwellian wavelength distributions (Part 1)
- FOCUS instrument was simulated for the wavelengths 2 Å, 4 Å and 6 Å (typical working range of FOCUS) – Part 2

# FOCUS Guide System – Part 1



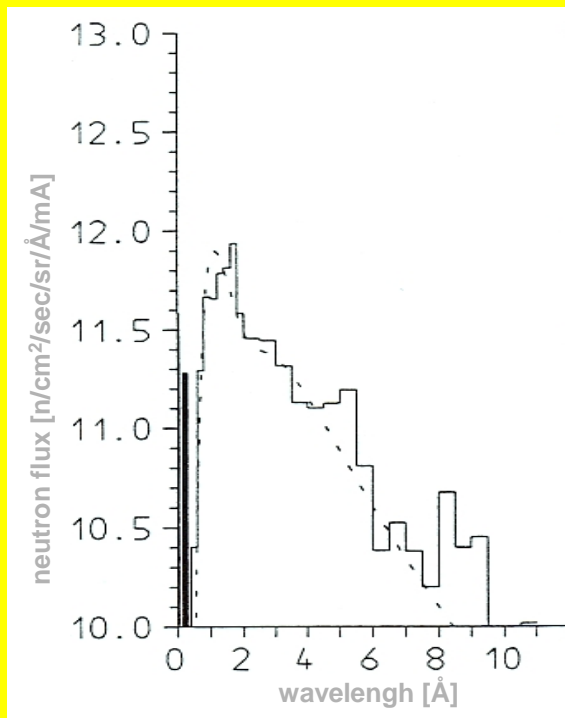
## Comparison of Intensities at Different Guide Positions for Wavelength Range 0.1 - 20 Å (flat wavelength distribution)

guide position	McStas	VITESS	deviation
1.77 m	1.000	1.000	
3.77 m	0.638	0.641	0.47 %
6.43 m	0.586	0.588	0.34 %
18.43 m	0.512	0.515	0.58 %
30.93 m	0.466	0.470	0.85 %
39.27 m	0.443	0.447	0.89 %
54.17 m	0.411	0.415	0.96 %
62.67 m	0.396	0.399	0.75 %
66.89 m	0.389	0.393	1.02 %
69.90 m	0.369	0.378	2.38 %

The calculated values from VITESS are slightly higher as in McStas.

## PSI - Cold Source Definition Parameters for Absolute Neutron Flux Calculations

raw data and their flux-Maxwellian fit function



$$f(\lambda)d\lambda = \sum_{i=0}^{i=1} I_i * 2 * \left(\frac{\lambda_{T_i}}{\lambda}\right)^4 \exp\left(-\frac{\lambda_{T_i}}{\lambda}\right) \frac{d\lambda}{\lambda}$$

Maxwellian distribution function

Two-Maxwellian parameter set for the cold source :

$$I_0 = 8.5 \cdot 10^{11} \text{ n/cm}^2/\text{sr}/\text{sec}/\text{mA}$$

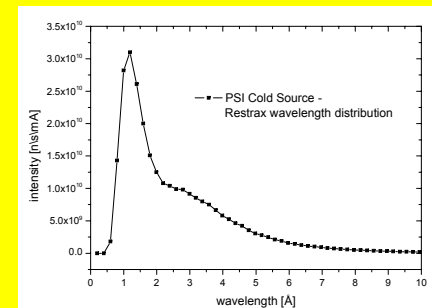
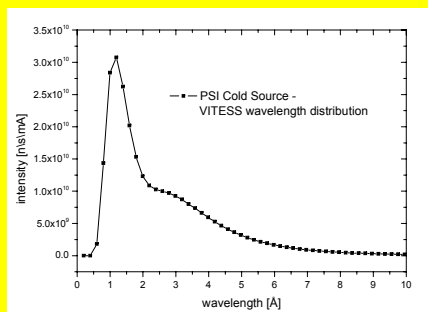
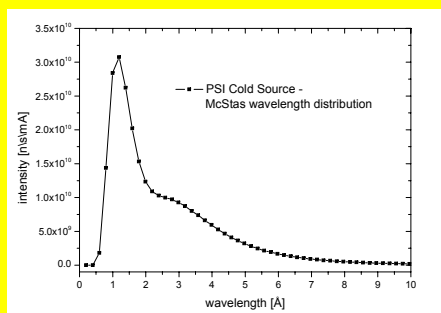
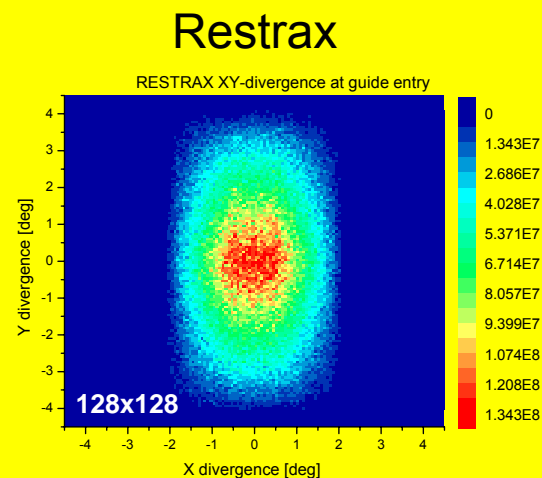
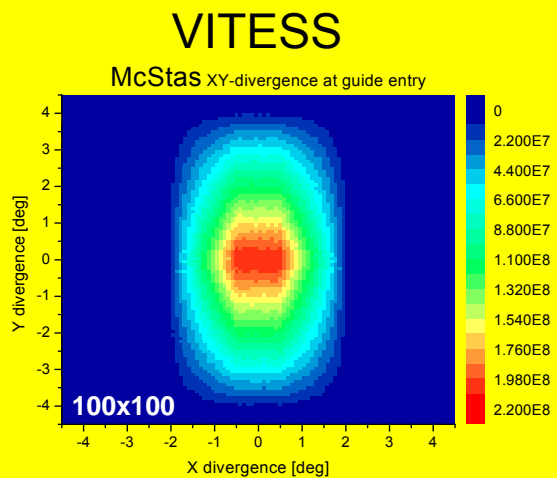
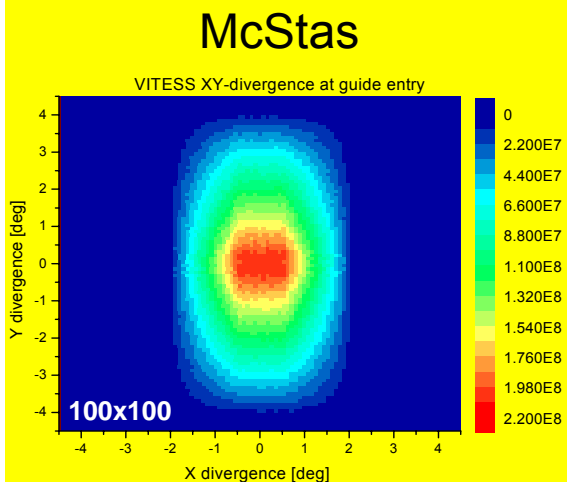
$$\lambda_{T0} = 1.79 \text{ \AA}$$

$$I_1 = 5.2 \cdot 10^{11} \text{ n/cm}^2/\text{sr}/\text{sec}/\text{mA}$$

$$\lambda_{T1} = 4.83 \text{ \AA}$$

Ref: F. Atchison, „Calculated neutron intensities for SINQ“, PSI report No. 98-03

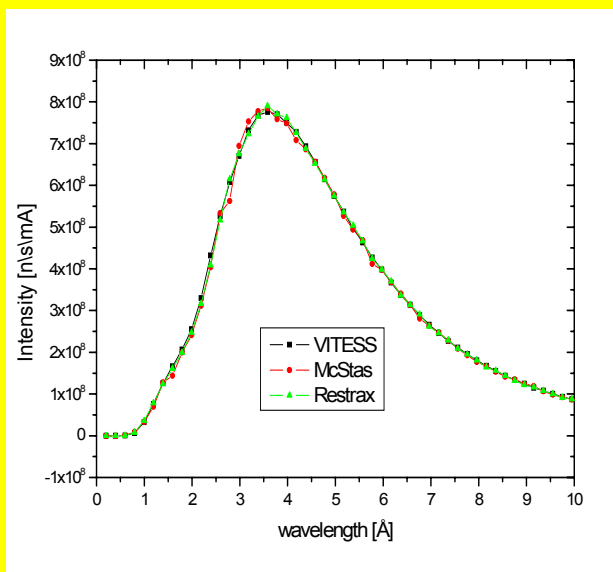
# McStas/VITESS/Restrax Input 1.77 m Position – Guide Entrance



## Comparison of Intensities at Different Guide Positions for Wavelength Range 0.1 - 20 Å

guide position	McStas [n/s]	VITESS [n/s]	Restrax [n/s]	Deviations (MV/MR/VR) [%]
1.77 m	2.829e+11 +/- 6.63e+07	2.829e+11 +/- 8.96e+07	2.818E+11 +/- 2.053E+08	0.00/0.4/0.4
3.77 m	7.487e+10 +/- 3.15e+07	7.508e+10 +/- 4.24e+07	7.471E+10 +/- 1.247E+08	-0.28/0.2/ 0.5
6.43 m	4.093e+10 +/- 2.02e+07	4.114e+10 +/- 2.68e+07	4.094E+10 +/- 9.741E+07	-0.51/0.0/ 0.5
18.43 m	2.375e+10 +/- 1.11e+07	2.409e+10 +/- 1.43e+07	2.389E+10 +/- 4.335E+07	-1.41/-0.6/0.8
30.93 m	2.038e+10 +/- 9.20e+06	2.062e+10 +/- 1.15e+07	2.057E+10 +/- 1.341E+07	-1.16/-0.9/0.2
39.27 m	1.932e+10 +/- 8.89e+06	1.955e+10 +/- 1.11e+07	1.947E+10 +/- 2.437E+07	-1.17/-0.8/0.4
54.17 m	1.778e+10 +/- 8.45e+06	1.799e+10 +/- 1.05e+07	1.794E+10 +/- 2.492E+07	-1.16/-0.9/0.3
62.67 m	1.705e+10 +/- 8.24e+06	1.725e+10 +/- 1.03e+07	1.716E+10 +/- 1.966E+07	-1.16/-0.6/0.5
66.89 m	1.672e+10 +/- 8.24e+06	1.691e+10 +/- 1.02e+07	1.683E+10 +/- 3.507E+07	-1.12/-0.6/0.5
69.90 m	1.593e+10 +/- 7.87e+06	1.623e+10 +/- 9.84e+06	1.617E+10 +/- 1.890E+07	-1.85/-1.5/0.4

## Comparison Measured and Simulated Absolute Neutron Flux for the FOCUS Guide System



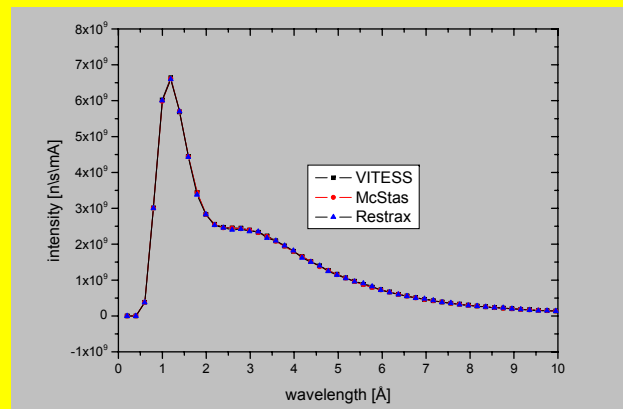
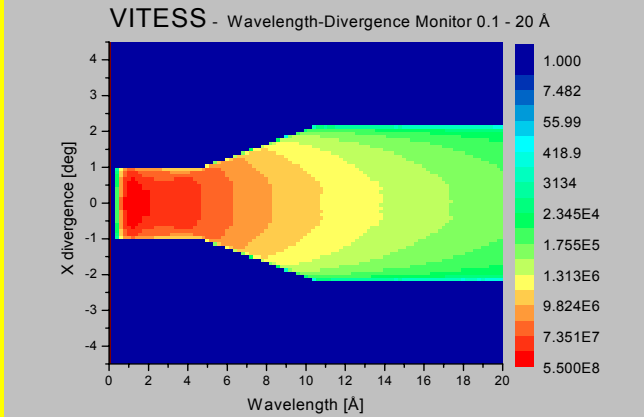
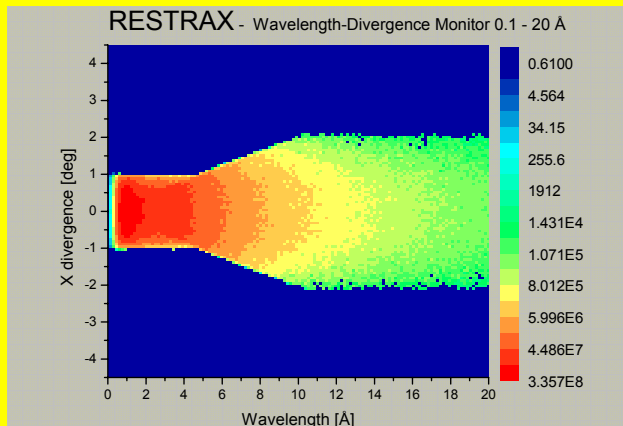
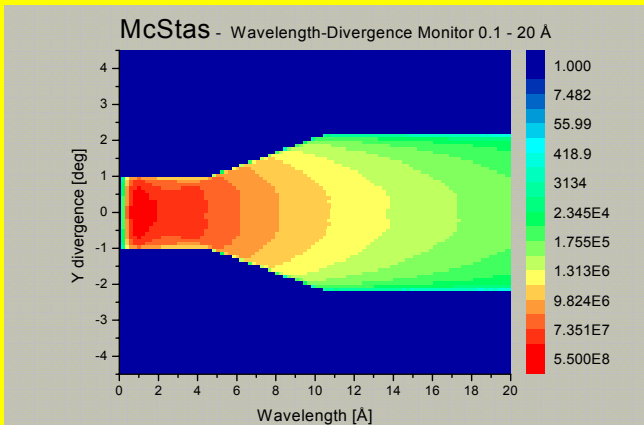
wavelength distributions at position 54.17 m

guide position	McStas $\Phi$ [n/cm <sup>2</sup> sec]	VITESS $\Phi$ [n/cm <sup>2</sup> sec]	Restrax $\Phi$ [n/cm <sup>2</sup> sec]	goild foil measurement $\Phi$ [n/cm <sup>2</sup> sec]
54.17 m	$2.96 \cdot 10^8$ (3.37%)	$3.00 \cdot 10^8$ (4.67 %)	$2.99 \cdot 10^8$ (4.43 %)	$2.86 \cdot 10^8$
62.67 m	$2.83 \cdot 10^8$ (10.60 %)	$2.87 \cdot 10^8$ (11.84 %)	$2.86 \cdot 10^8$ (11.53 %)	$2.53 \cdot 10^8$

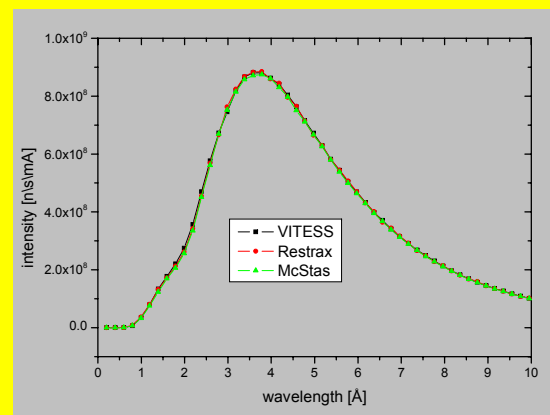
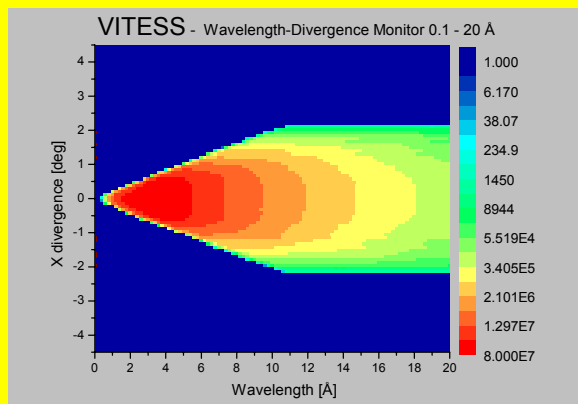
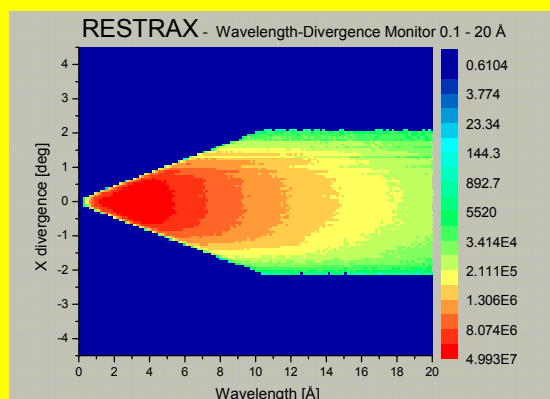
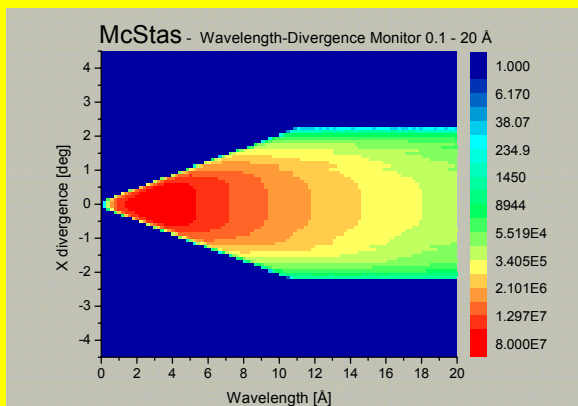
\*neutron flux is given for 1 mA SINQ current (circular target)



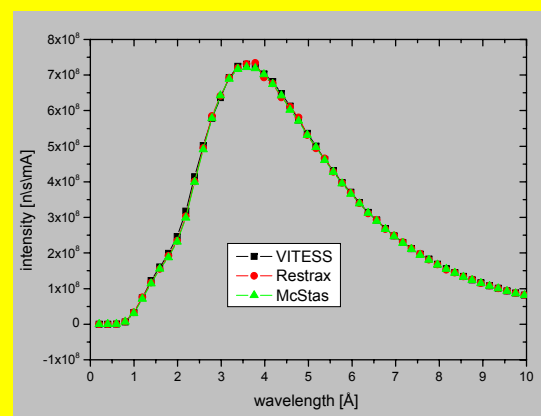
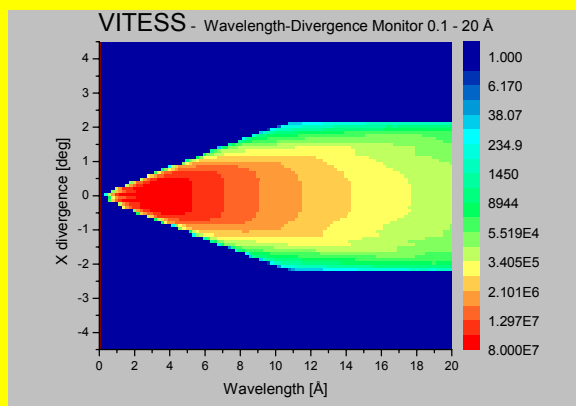
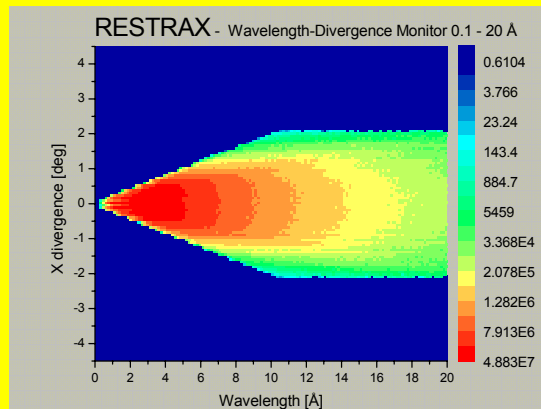
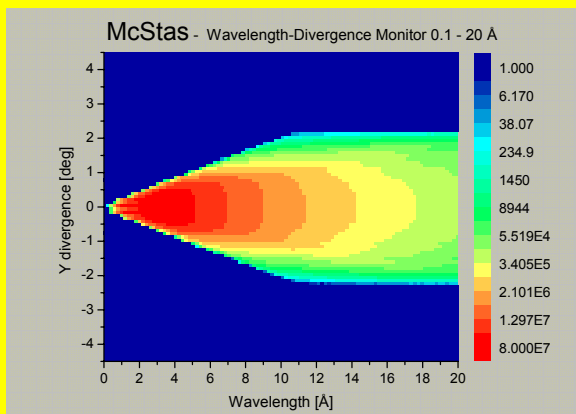
# Comparison of Wavelength-Divergence and Wavelength distribution at Position 3.77 m for the Wavelength Range of 0.1 - 20 Å



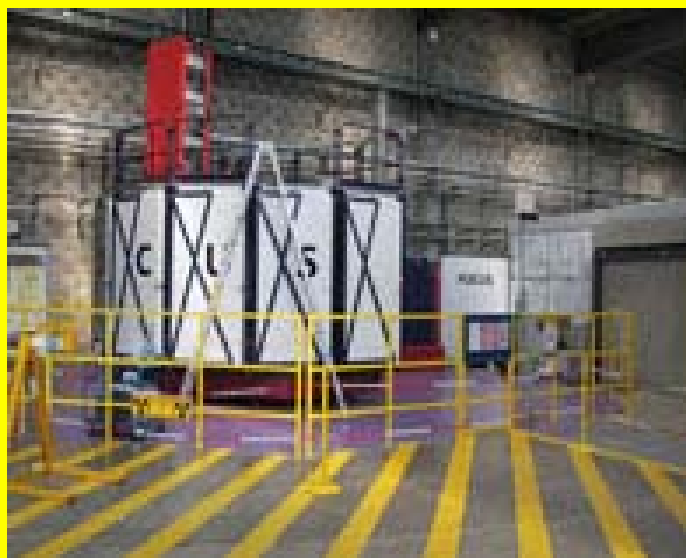
# Comparison of Wavelength-Divergence and Wavelength-distribution at Position 30.93 m for the Wavelength Range of 0.1 - 20 Å



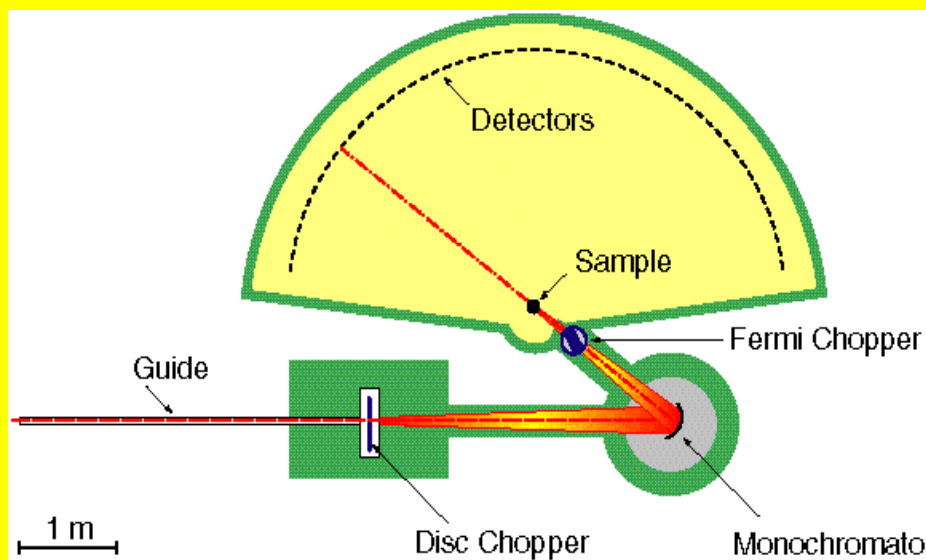
# Comparison of Wavelength-Divergence and Wavelength-distribution at Position 66.89 m for the Wavelength Range of 0.1 - 20 Å



# FOCUS Instrument simulations – Part 2

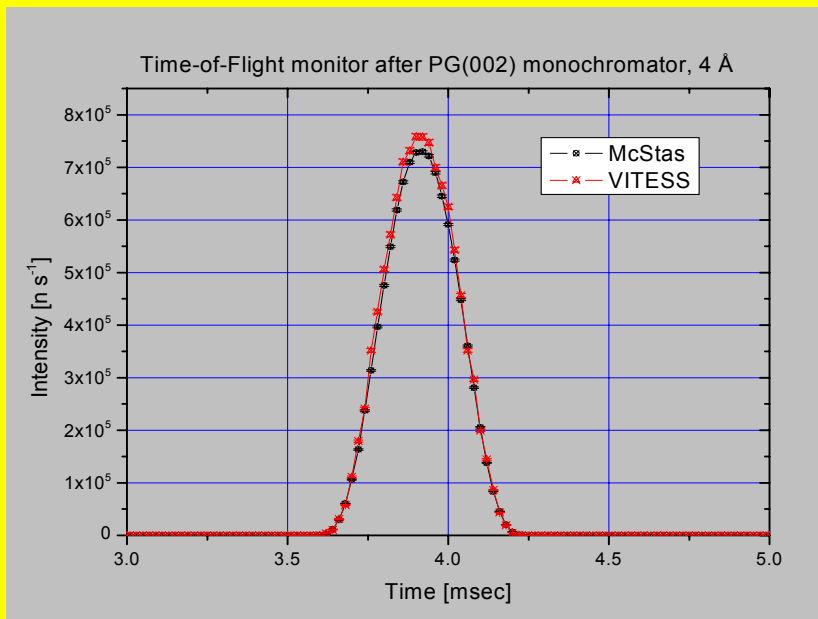
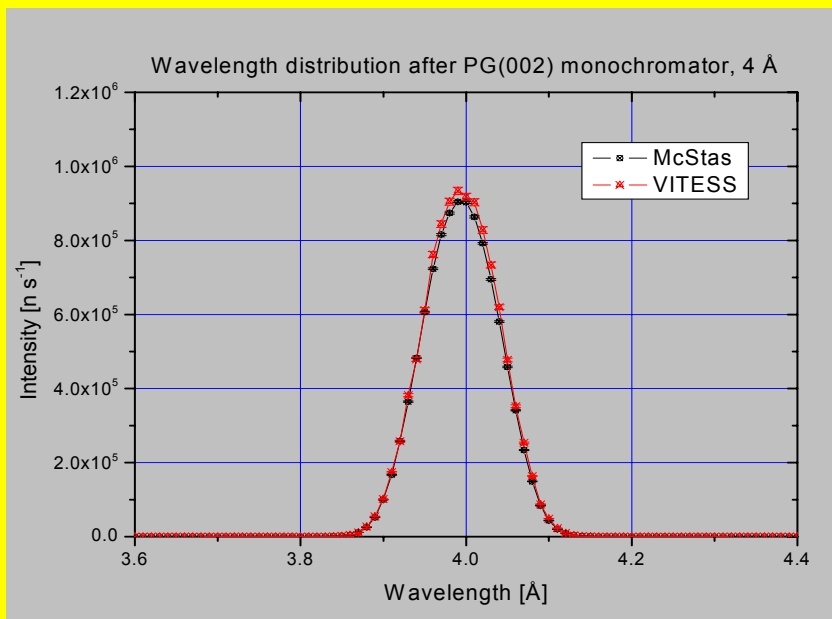


**View on FOCUS**



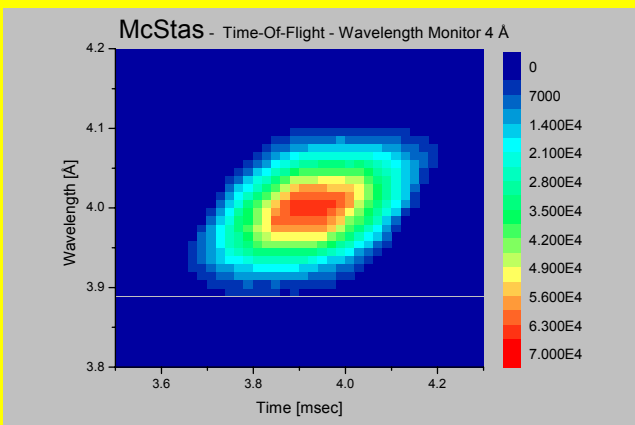
**Schematic design of the time-of flight spectrometer FOCUS**

Comparison of Time-of-Flight and Wavelength-Distribution  
Monitors in front of Fermi-Chopper 0.94 m behind  
Monochromator for 4 Å

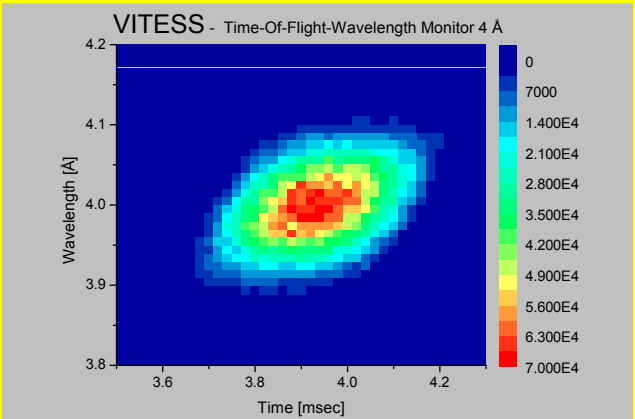
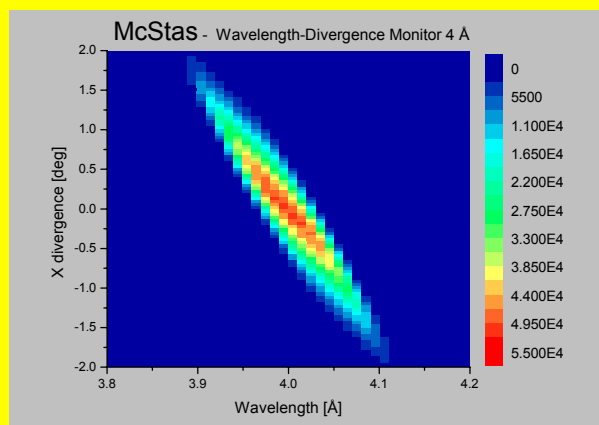


wavelength	McStas	VITESS	deviation
2 Å	4.050·10 <sup>6</sup> n/s	4.330·10 <sup>6</sup> n/s	6.67 %
4 Å	1.057·10 <sup>7</sup> n/s	1.097·10 <sup>7</sup> n/s	3.71 %
6 Å	2.631·10 <sup>6</sup> n/s	2.698·10 <sup>6</sup> n/s	2.51 %

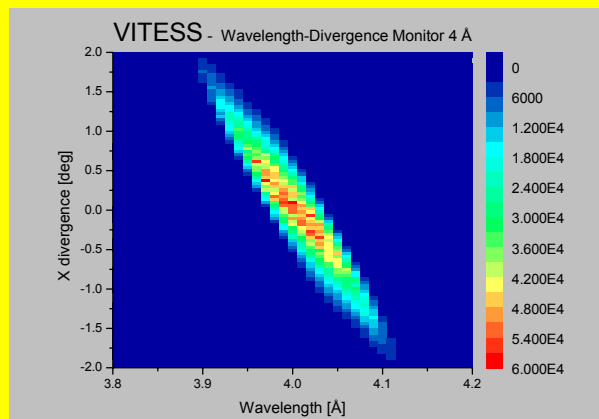
Comparison of Position-Divergence and time-of-flight-  
Wavelength Monitors in front of Fermi-Chopper 0.94 m behind  
Monochromator for 4 Å



McStas

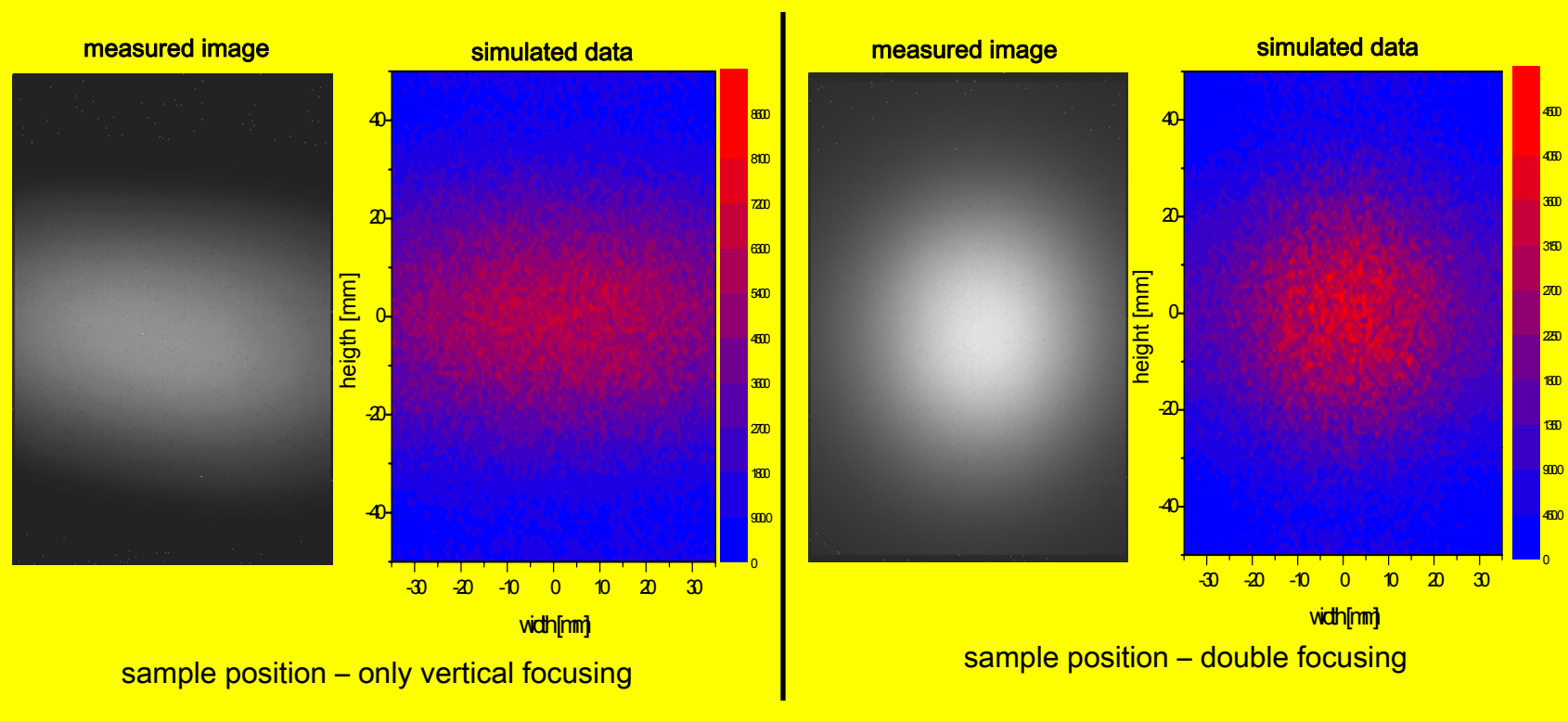


VITESS

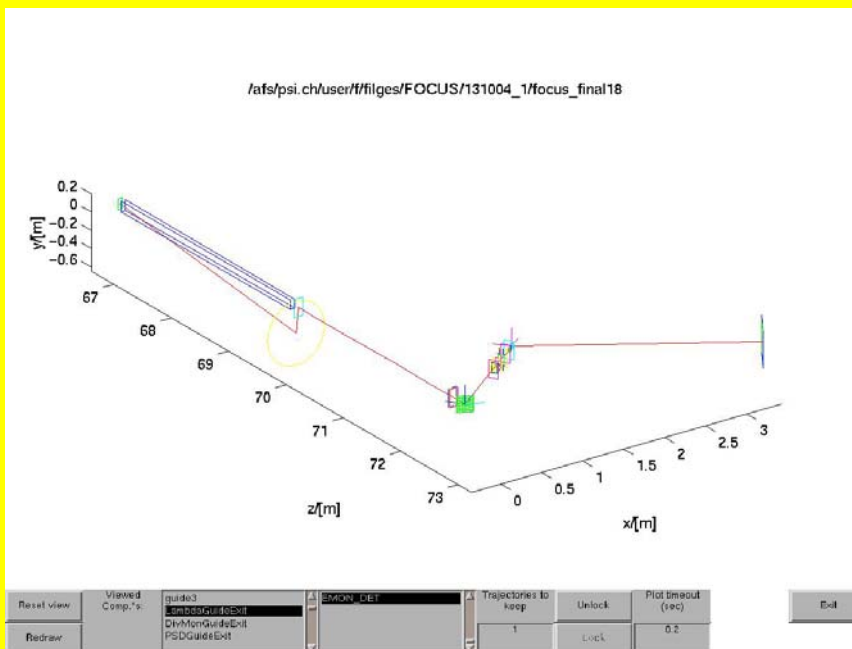


# Comparison of Beam Profiles

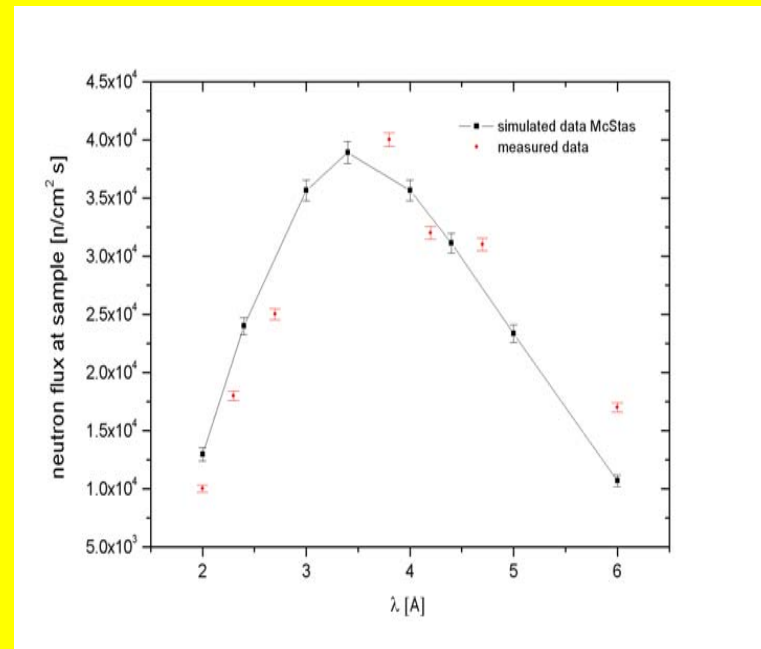
- measurements were performed with a neutron imaging camera 95 x 65 mm (HxW)



# Comparison of neutron flux at sample position



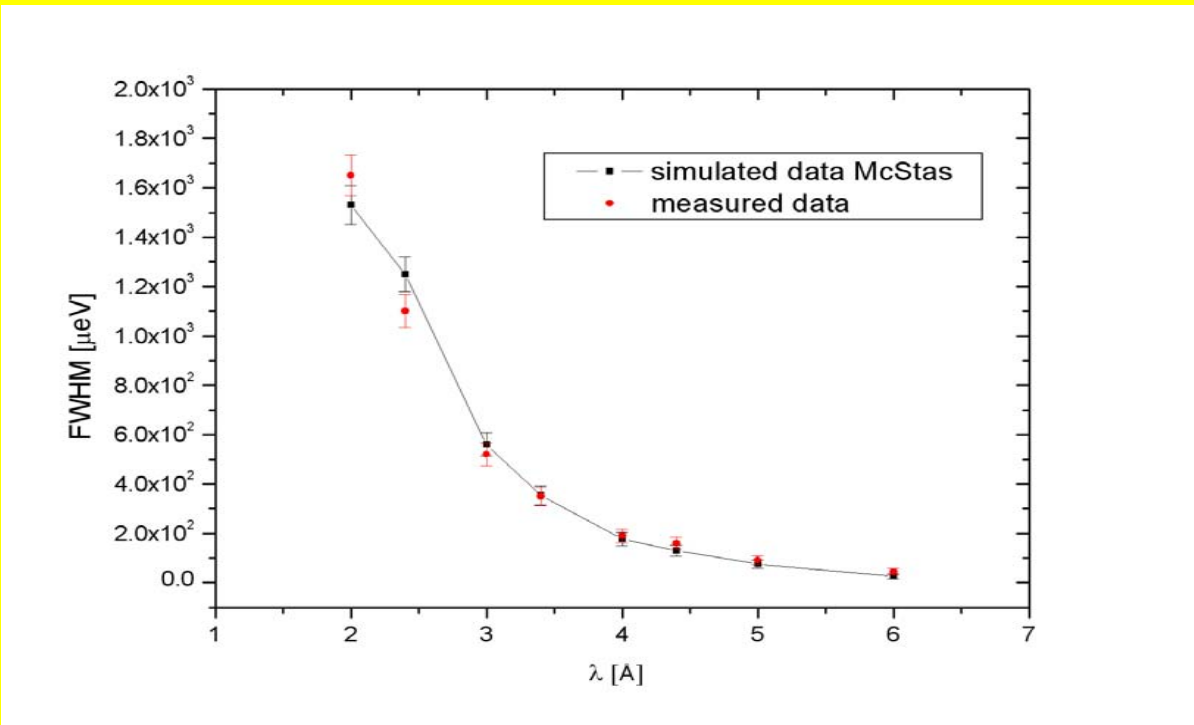
McStas – Matlab plot of FOCUS input file



Measured and simulated neutron flux at sample position (McStas)



# Comparison of Energy Resolution at Sample Position



Energy resolution for the PG002 monochromator

# Summary

- the guide intercomparison shows nearly perfect consistency between all three used packages (McStas,VITESS,Restrax)
- the measured neutron flux values are differ only in range of 5 -10 %
- after the monochromator the differences between McStas and VITESS are slightly higher (small wavelength range)
- measurements at sample are agree very well with simulated McStas data (VITESS simulations will be done soon)