McStas

Validation of velocity selector, guide and source components in McStas

Klaus Lieutenant

Methods

- Test methods
  - internal test:
    - following neutrons through the instrument
    - check by analytical calculations (using calculator, Excel, ...)
  - external test (black box test):
    - use of a model instrument
    - comparison of output with
      - analytical functions or
      - cross-check with another package
  - integration test:
    - simulation of a whole beamline or instrument
    - comparison of the results obtained by different components / packages

Components checked

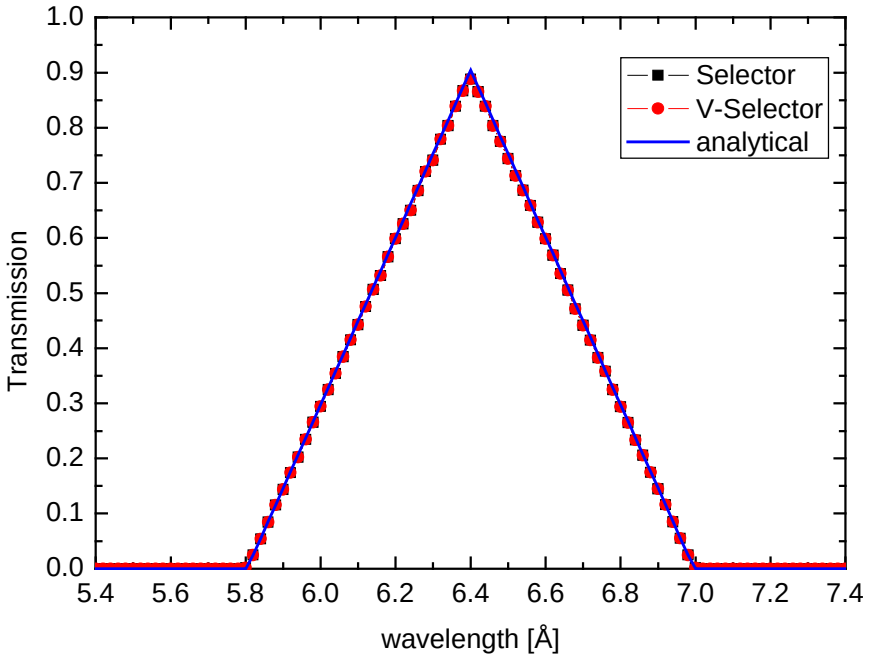
- Velocity selectors
  - Components
    - V-selector (K. Lefmann)
    - Selector (P. Link)
  - External test (compared to analytical functions - own calculations)
- Sources
  - Component
    - Source_gen (E. Farhi)
  - Methods
    - external test (compared to other simulations)
    - integration test
- Guides
  - Components
    - Guide (K. Nielsen)
    - Guide_gravity (E. Farhi)
  - Test methods
    - internal test (calculation of individual trajectories)
    - integration test

Velocity Selector test 1: non-diverg. beam

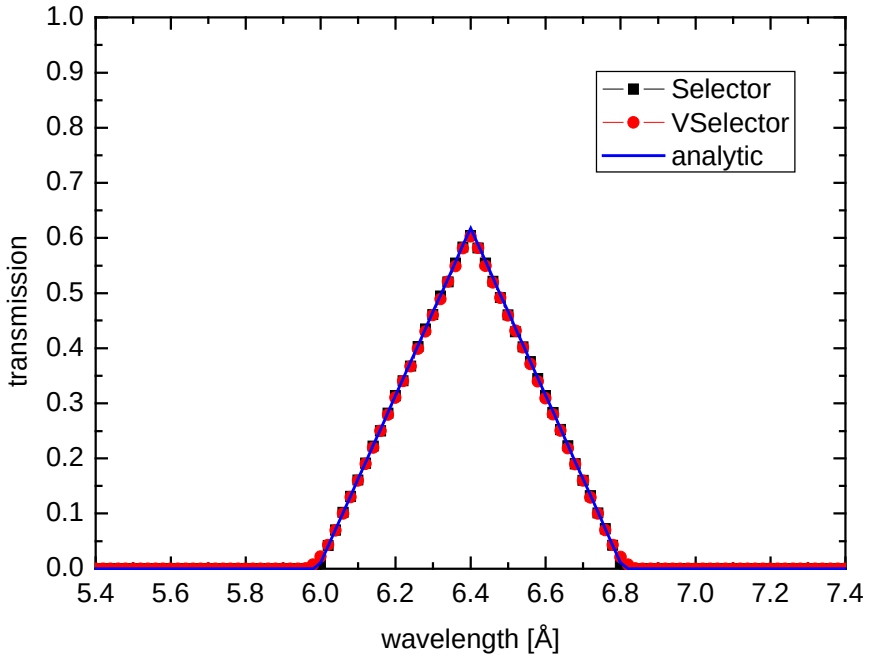
- Configuration 1
  - Source
    - 10 x 10 mm²
    - average wavelength 6.4 Å
    - no divergence
    - Component 'Source_div' in new option 'wavelength uniform'
  - Velocity selector
    - apertures 10 x 10 mm²
    - 20000 rpm
    - twist angle 48.534 deg
    - distance aperture - axle: 30, 60, 90, 120, 150, 180 mm
    - 72 blades of 1 mm thickness
    - length 250 mm
      (radius is assumed to be infinite in the components)
  - Monitors
    - wavelength monitors before and after the velocity selector
    - Component: 'Monitor_nD' with centered x-values

Test 1a: transmission P(λ)

120 mm distance from axle



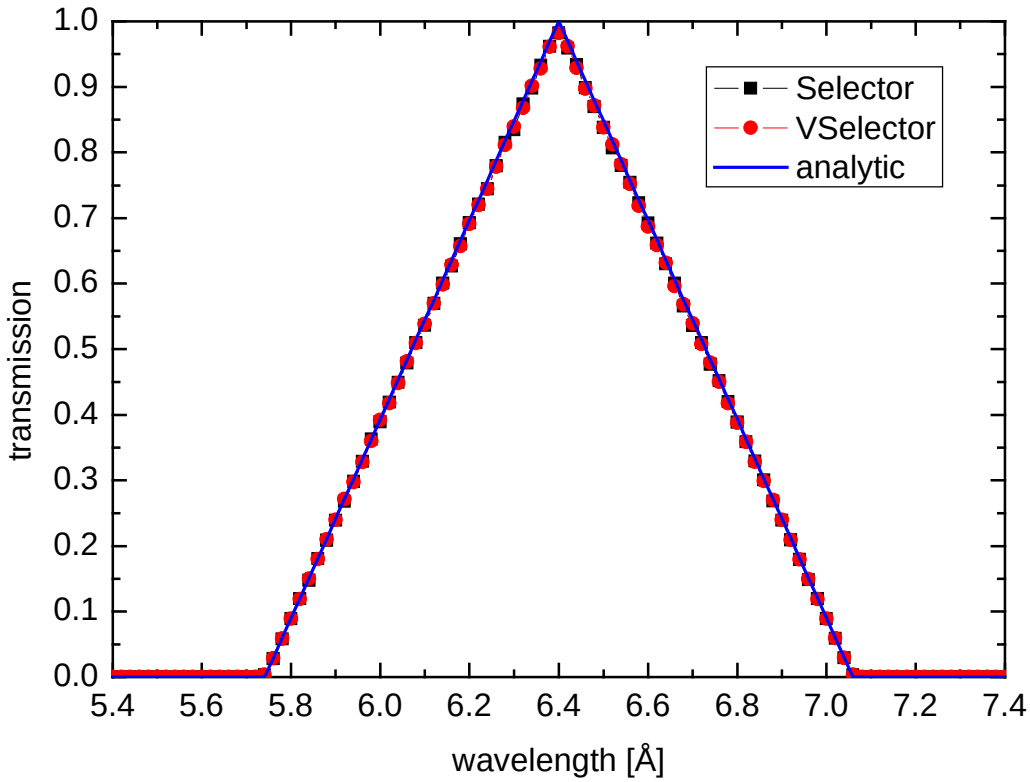
30 mm distance from axle



- Check 1a: transmission for different distances axle - guide centre
- Result for both components and all examined distances
  - average wavelength correct
  - width (in wavelength) correct
  - (triangular) shape correct
  - maximal transmission correct

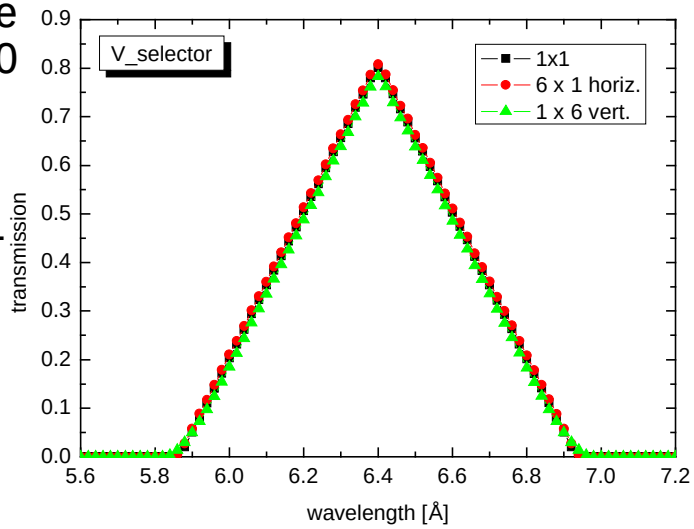
Test 1b: infinitely thin blade

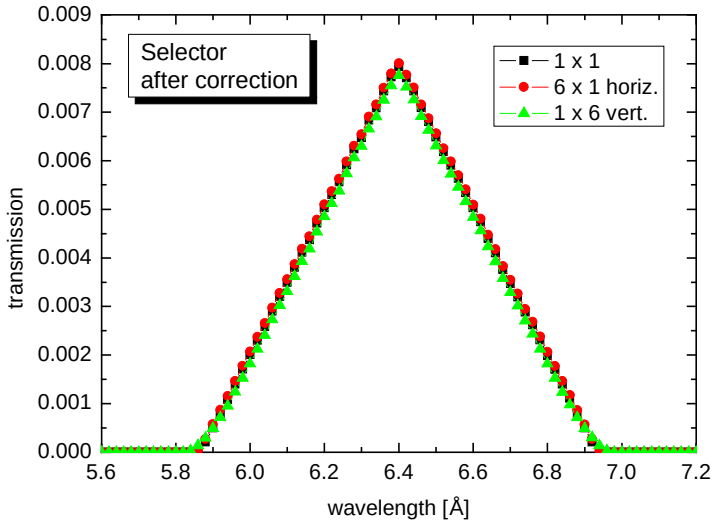
- Idea
  - Transmission should be 1 for the optimal wavelength if blades are infinitely thin (and the beam is not divergent)
- Result
  - This is found for both components

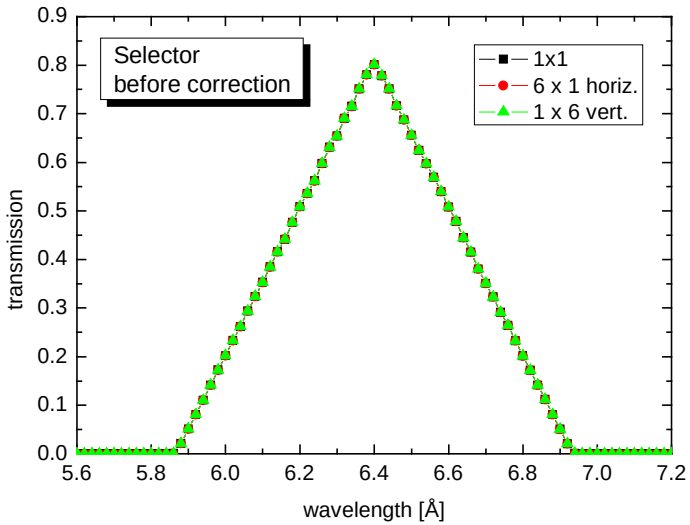


Check 1c: different window shape

- Idea:
  - a long, narrow window straightened towards the axle should reduce the transmission; the same window 90 deg rotated should increase the transmission
- Simulation:
  - 6 x 1 cm^2 and 1 x 6 cm^2 used in comparison to 1 x 1 cm^2 window
- Results:
  - Selector before correction no differences - failed
  - V-Selector and selector after correction: differences in the right direction and of a realistic size - correct







Check 1d,e: rotation direction and '2nd frame'

- Idea of check 1d:
  - Inversion of direction of rotation or twist angle should block all neutrons:
- Result for both components:
  - transmission gets 0 for a wrong combination of twist angle and direction of rotation - correct (s. table)

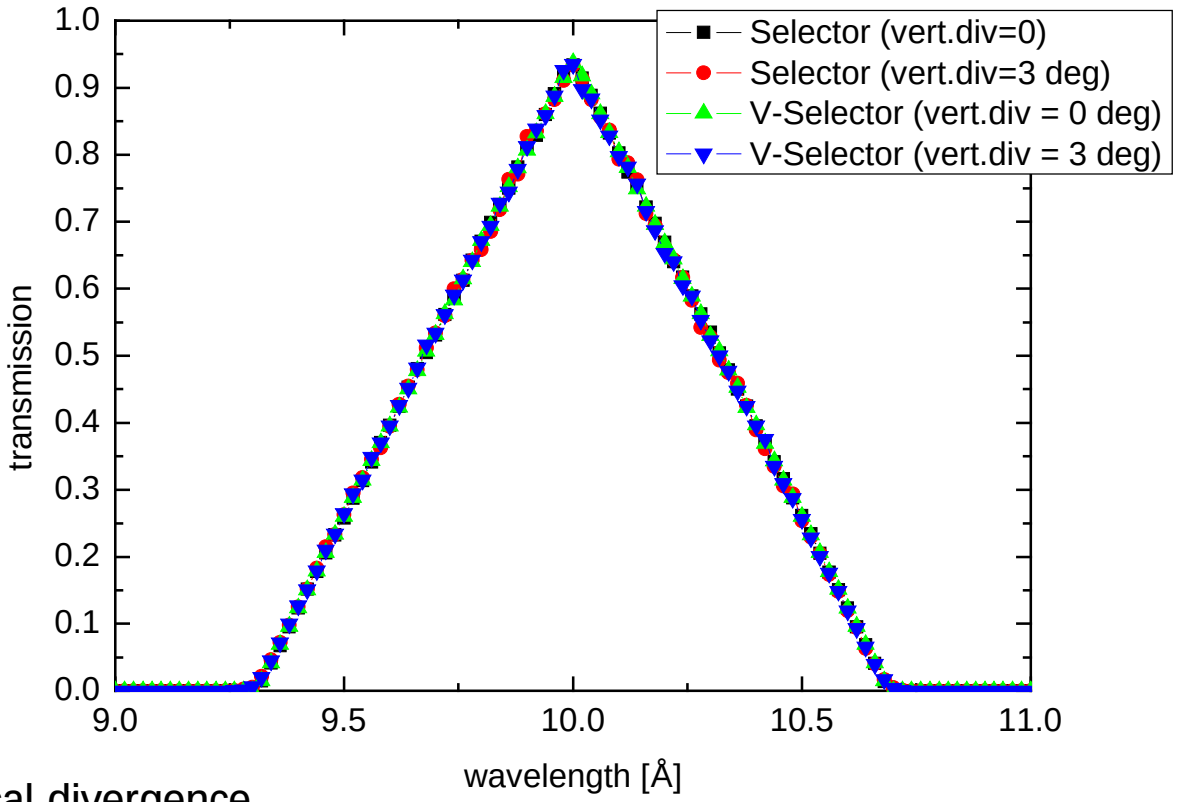
		direction	of rotation
		+	-
twist	+	transmission	no transm.
angle	-	no transm.	transmission

- Idea of check 1e:
  - The 'Selector' checks if the neutron is in the same channel at entrance and exit, this could also be the case after a rotation of (α + 360 deg) instead of α, which would result in a (not existing) transmission of long wavelengths - a second frame
- Result :
  - Selector: no second frame found - correct
  - V-Selector: not checked as it works with an analytic formula; therefore this effect cannot appear

Velocity selector test 2: divergent case

- Configuration 2
  - Source
    - size adapted to divergence
    - average wavelength 10 Å
    - divergence in horizontal or vertical direction
    - Component 'Source_div' in new option 'wavelength uniform'
  - Velocity selector
    - apertures 10 x 10 mm^2
    - 12000 rpm
    - twist angle 54.600 deg
    - distance aperture - axle: 40, 100 mm
    - 90 blades of 0.4 mm thickness
    - length 300 mm
      (radius is assumed to be infinite in the components)
  - Monitors
    - wavelength and 1-dimensional divergence monitors before and after the velocity selector
    - Component: 'Monitor_nD' with centered x-values

Test 2a: vertical divergence

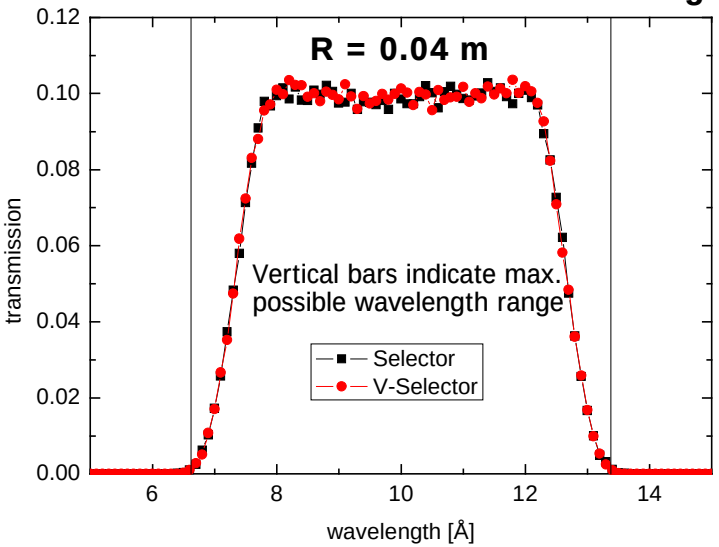


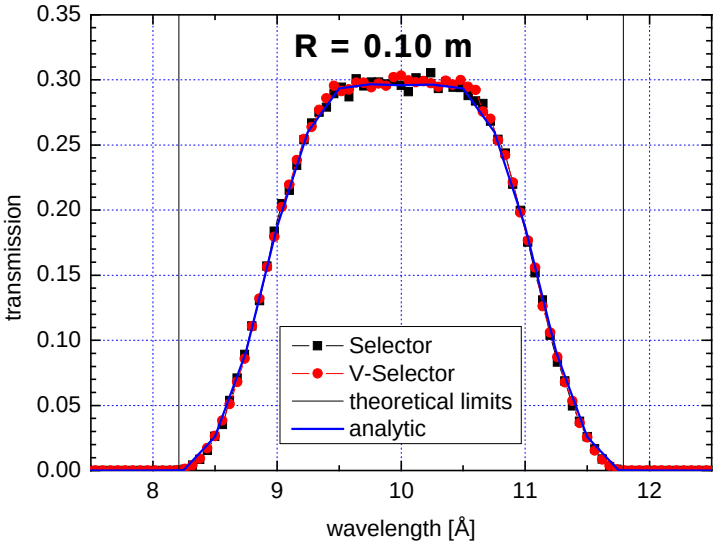
- Configuration:
  - 0 deg and 3 deg vertical divergence
- Expected:
  - no incluence of vertical divergence
- Results:
  - no influence of vertical divergence for both components

Test 2b: wavelength range

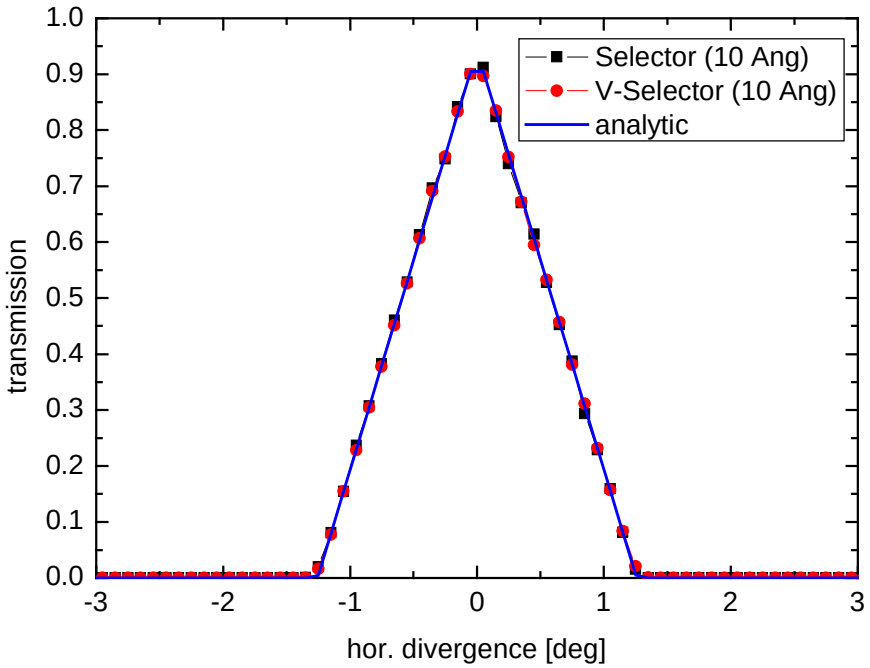
- Configuration 2b:
  - 2 deg horizontal divergence
- Results for both components:
  - minimal and maximal wavelength correct
  - transmission as a function of wavelength correct (only checked for 0.10 m distance between axle and guide centre).

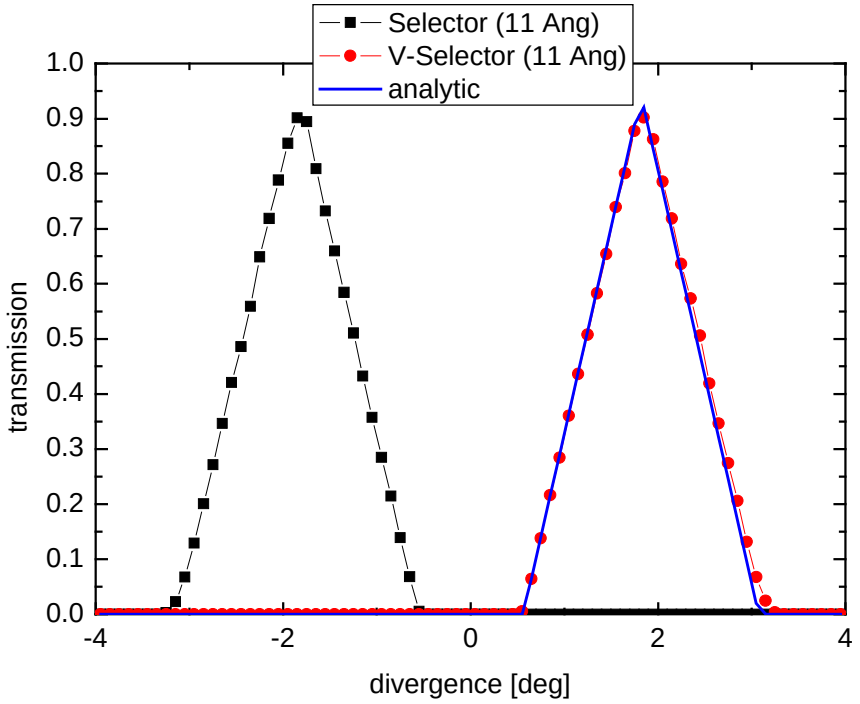
Transmission P as a function of wavelength for different distances axle - centre of guide





Test 2c: transmission as a fct. of diverg.





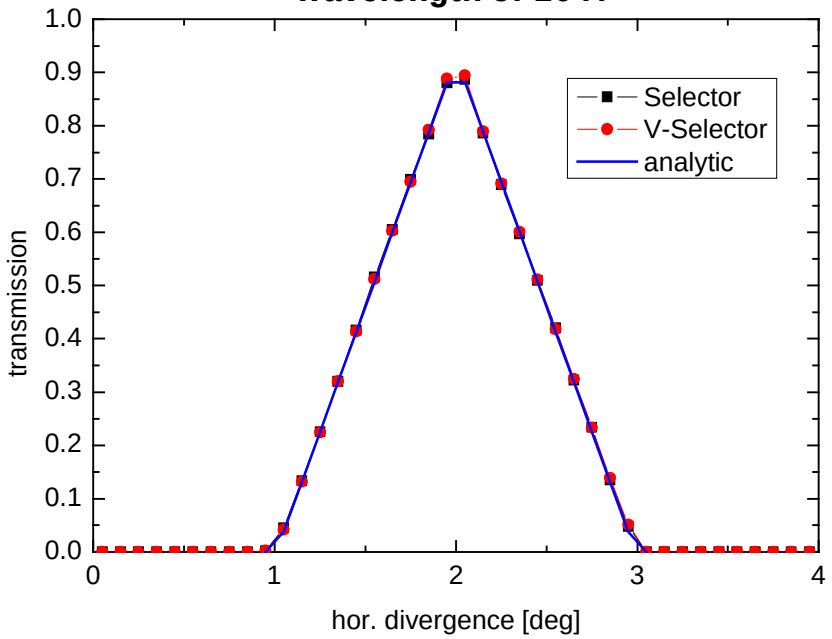
- Configuration 2c:
  - 3.5 deg horizontal divergence
  - fixed wavelengths 9, 10, 11 Å
- Result:
  - 'V-selector': shift of optimal wavelength correct
  - 'Selector': shape correct, shift into the other direction
  - transmission as a function of wavelength correct (for both packages)

Velocity selector test 3: tilted

Shift of transmitted wavelength range for non-divergent beam through a tilted selector

	kink [deg]	-2	-1	0	1	2
analytical	min. wavelength [Ang]	10.694	10.007	9.320	8.633	7.946
	max. wavelength [Ang]	12.054	11.367	10.680	9.993	9.306
	max. transmission	0.928	0.928	0.928	0.928	0.928
	average transmission	0.0789	0.0789	0.0789	0.0789	0.0789
V-Selector	min. wavelength [Ang]	10.56	10.00	9.28	8.56	7.84
	max. wavelength [Ang]	12.16	11.44	10.72	10.00	9.36
	max. transmission	0.866	0.909	0.900	0.899	0.896
	average transmission	0.0780	0.0781	0.0782	0.0781	0.0781
Selector	min. wavelength [Ang]	10.64	10.00	9.36	8.56	7.84
	max. wavelength [Ang]	12.16	11.44	10.64	10.00	9.36
	max. transmission	0.862	0.909	0.902	0.878	0.861
	average transmission	0.0781	0.0782	0.0782	0.0781	0.0780
		2	1	0	-1	-2

Transmission as a function of divergence for fixed wavelength of 10 Å

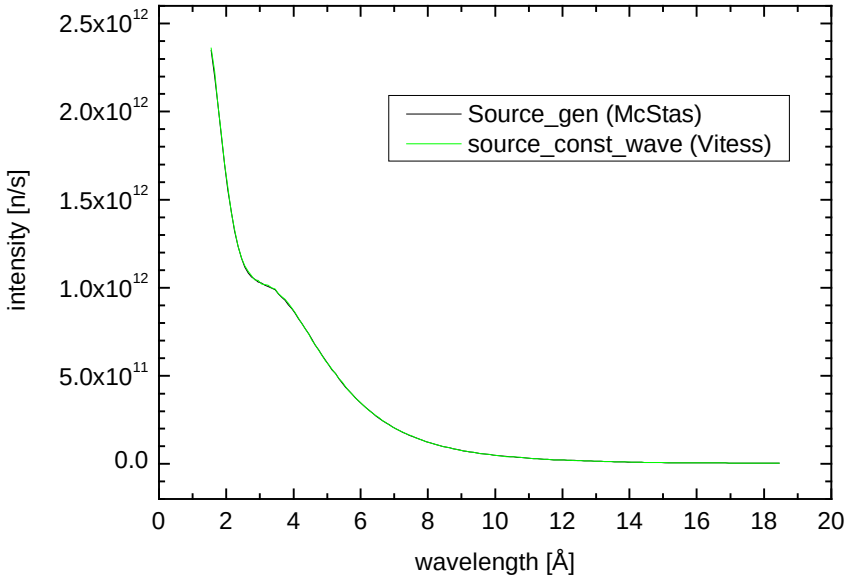


- Configuration 3
  - as configuration 2 except R = 0.08 m
  - whole velocity selector tilted by -2, -1, 0, 1, 2 deg
- Result for both components
  - non-divergent case: shift of wavelength and transmission correct (s. Table), but again into wrong direction for 'Selector'
  - divergent case: maximal transmission of dedicated wavelength (10 Å) for tilt angle - as expected

External test: 'Source_gen'

- Simulation:
  - Part of the IN14 simulation repeated by H. Bordallo and T. Seydel (s. below)
  - Source_gen (McStas) and source_const_wave (VITESS) used
  - wavelength range examined: 1.5 - 18.5 Å
  - 3 Maxwellians (old description of HCS)
  - 42 cm diameter
  - window of 60 x 120 mm^2 (W x H) in a distance of 2.155 m (H53)

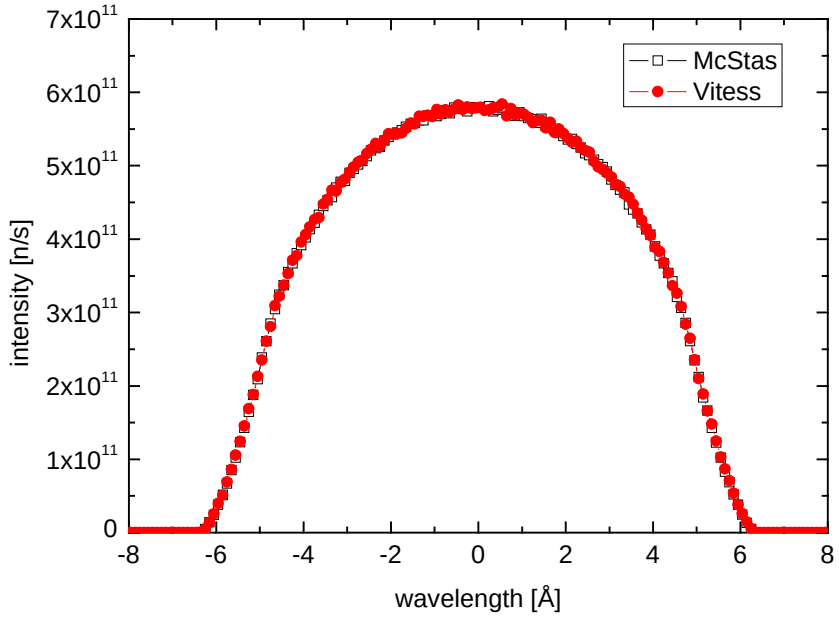
Flux at guide exit in McStas and VITESS



- Result:
  - intensities as a function of wavelength nearly identical

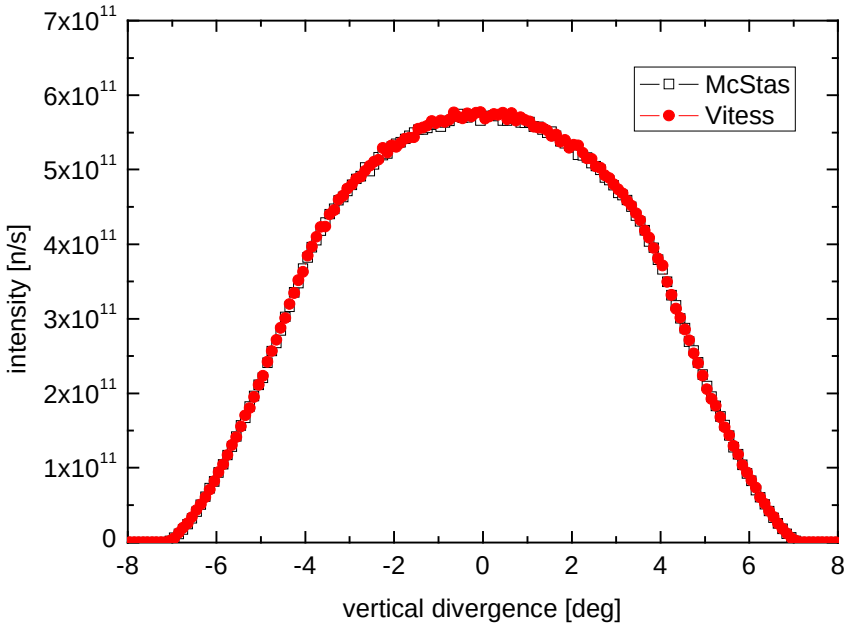
Source_gen: divergence distribution

Maximal theoretical value: 6.35°



Horizontal divergence averaged over window in McStas and VITESS

Maximal theoretical value: 7.14°



Vertical divergence averaged over window in McStas and VITESS

- Result:
  - Distribution of divergence identical, both in horizontal and vertical direction
  - Maximal values correct

Internal tests of component 'Guide'

- Parameters checked
  - position of reflection
  - velocity and flight direction after reflections
  - q value
  - loss of weight by reflection
- Guide types checked
  - constant cross-section
  - converging
  - diverging
- Result
  - Guide works perfectly (without corrections)

Component	option	Test	Result	Errors / Bugs
Guide	straight	position of reflection	o.k.	
		velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	converging	position of reflection	o.k.	
		velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	diverging	position of reflection	o.k.	
		velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	

Internal tests of component 'Guide_gravity'

Component	option	Test	Result	Errors / Bugs
Guide_grav	G = 0.0	position of reflection	o.k.	
	straight	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	G = 0.0	position of reflection	o.k.	
	converging	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	G = 0.0	position of reflection	o.k.	
	diverging	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
Guide_grav	G = -9.80665	position of reflection	o.k.	
	straight	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	G = -9.80665	position of reflection	o.k.	
	converging	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
	G = -9.80665	position of reflection	o.k.	
	diverging	velocity after refl.	o.k.	
		q value	o.k.	
		loss of weight	o.k.	
Guide_grav	G = -9.80665	position of reflection	o.k.	
	converging	velocity after refl.	o.k.	
	odd no of channels	q value	o.k.	
		loss of weight	o.k.	
	G = -9.80665	position of reflection	o.k.	
	converging	velocity after refl.	o.k.	
	even no of channels	q value	o.k.	
		loss of weight	o.k.	

- Parameters
  - same as with 'Guide'
- Conditions
  - in absence of gravity
  - with gravity effect
- Guides
  - constant cross-section
  - converging guides
  - diverging guides
  - channeled converging (only with gravity)
- Not checked
  - waviness
  - chamfers
- Result
  - After corrections Guide_gravity works fine

Example: straight guide, with gravity

after reflection	wall	t [s]	x [mm]	y [mm]	z [m]	v_x [m/s]	v_y [m/s]	v_z [m/s]	q [1/Ang]	p
Guide_grav										
intial	entrance	0.000	-12.50	-2.057	0.00	0.625	1.049	250.00		1.0000
1	top	0.030	6.25	25.000	7.50	0.625	-0.755	250.00	0.002397	0.9900
2	left	0.060	25.00	-2.057	15.00	-0.625	-1.049	250.00	0.001985	0.9801
3	bottom	0.080	12.50	-25.000	20.00	-0.625	1.245	250.00	0.003956	0.9703
4	top	0.130	-18.75	25.000	32.50	-0.625	-0.755	250.00	0.002397	0.9606
5	right	0.140	-25.00	16.962	35.00	0.625	-0.853	250.00	0.001985	0.9510
	exit	0.160	-12.50	-2.057	40.00	0.625	-1.049	250.00		
THEORY										
intial	entrance	0.000	-12.50	-2.057	0.00	0.625	1.049	250.00		1.0000
1	top	0.030	6.25	25.000	7.50	0.625	-0.755	250.00	0.002397	0.9900
2	left	0.060	25.00	-2.057	15.00	-0.625	-1.049	250.00	0.001985	0.9801
3	bottom	0.080	12.50	-25.000	20.00	-0.625	1.245	250.00	0.003956	0.9703
4	top	0.130	-18.75	25.000	32.50	-0.625	-0.755	250.00	0.002397	0.9606
5	right	0.140	-25.00		35.00	0.625		250.00	0.001985	0.9510
	exit	0.160	-12.50	-2.057	40.00	0.625	-1.049	250.00		
length [m]	40.00									
width [mm]	50.0									
height [mm]	50.0									
speed [m/s]	250	15.824	Ang							

Integrative test (ILL beamline)

- Motivation
  - Simulations with McStas and VITESS performed by Heloisa Bordallo
  - Discrepancies found by her between these simulations
- Test
  - VITESS simulation (practically) left as it was done by her
  - Simulation then transferred to McStas for comparison

Parts of the beamline	McStas components	VITESS
source	source_gen	source_const_wave
free flight path	source_gen	source_const_wave
horizontally converging guide	Guide / Guide_gravity	Guide
2 horizontally diverging guides	Guide / Guide_gravity	Guide
2 curved guide	Guide_curved	Guide
straight guide	Guide / Guide_gravity	Guide
converging guide	Guide / Guide_gravity	Guide

- Simulation parameters:
  - Wavelength range: 5 - 7 Å
  - flux: 1×10^{13} n/(cm^2 s str) (for whole λ range)
  - Maxwellian distribution of 50 K

Overall results

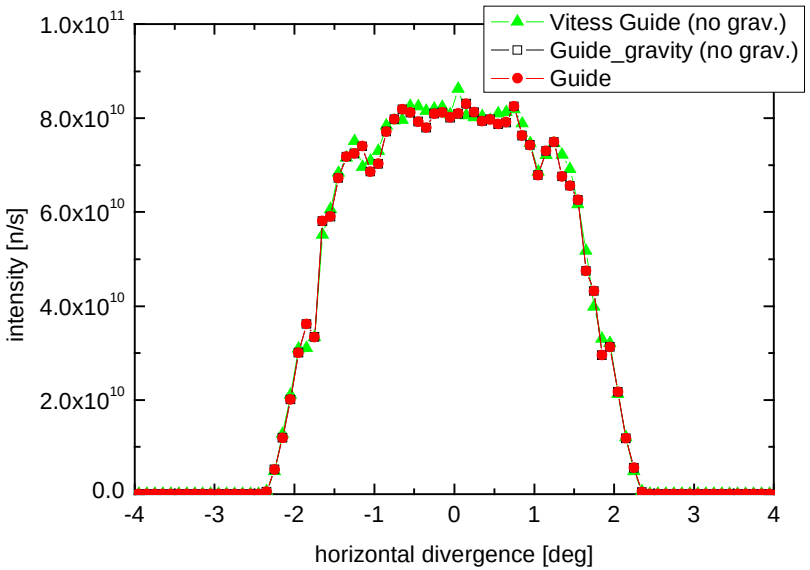
- First run
  - Wrong results with the actual version of Guide_gravity
- After corrections
  - Same flux for 'Guide', 'Guide_gravity' and the same instrument in VITESS

H112			6 Ang											
mon	after section	position [m]	intensity [n/s}			events	intensity [n/s}			events	intensity [n/s}			events
NO GRAVITY														
			Guide				Guide_gravity				Vitess Guide			
0		2.33	2.384E+14	+/-	7.68E+10	1.10E+07	2.384E+14	+/-	7.68E+10	1.10E+07	2.384E+14	+/-	7.68E+10	1.10E+07
1	hor. conv.	5.50	1.686E+13	+/-	1.93E+10	2.20E+06	1.686E+13	+/-	1.93E+10	2.20E+06	1.693E+13	+/-	1.93E+10	1.39E+06
2	hor. div. 1	7.78	1.372E+13	+/-	1.70E+10	2.19E+06	1.372E+13	+/-	1.70E+10	2.19E+06	1.379E+13	+/-	1.71E+10	1.34E+06
3	hor. div. 2	17.53	1.209E+13	+/-	1.56E+10	2.19E+06	1.209E+13	+/-	1.56E+10	2.19E+06	1.217E+13	+/-	1.57E+10	1.34E+06
5	curved	33.39	1.144E+13	+/-	1.51E+10	2.19E+06	1.144E+13	+/-	1.51E+10	2.19E+06	1.099E+13	+/-	1.46E+10	1.32E+06
6	straight	93.39	8.714E+12	+/-	1.25E+10	2.17E+06	8.713E+12	+/-	1.25E+10	2.17E+06	8.606E+12	+/-	1.24E+10	1.11E+06
7	focussing	100.39	2.796E+12	+/-	7.18E+09	2.00E+05	2.796E+12	+/-	7.18E+09	2.00E+05	2.827E+12	+/-	7.23E+09	1.87E+05
GR AVITY														
							Guide_gravity				Vitess Guide			
0		2.33					2.384E+14	+/-	7.68E+10	1.10E+07	2.384E+14	+/-	7.68E+10	1.10E+07
1	hor. conv.	5.50					1.686E+13	+/-	1.93E+10	2.20E+06	1.693E+13	+/-	1.93E+10	1.39E+06
2	hor. div. 1	7.78					1.372E+13	+/-	1.70E+10	2.19E+06	1.379E+13	+/-	1.71E+10	1.34E+06
3	hor. div. 2	17.53					1.209E+13	+/-	1.56E+10	2.19E+06	1.217E+13	+/-	1.57E+10	1.33E+06
5	curved	33.39					1.144E+13	+/-	1.51E+10	2.19E+06	1.098E+13	+/-	1.46E+10	1.32E+06
6	straight	93.39					8.712E+12	+/-	1.25E+10	2.17E+06	8.605E+12	+/-	1.24E+10	1.11E+06
7	focussing	100.39					2.795E+12	+/-	7.18E+09	2.00E+05	2.829E+12	+/-	7.23E+09	1.87E+05

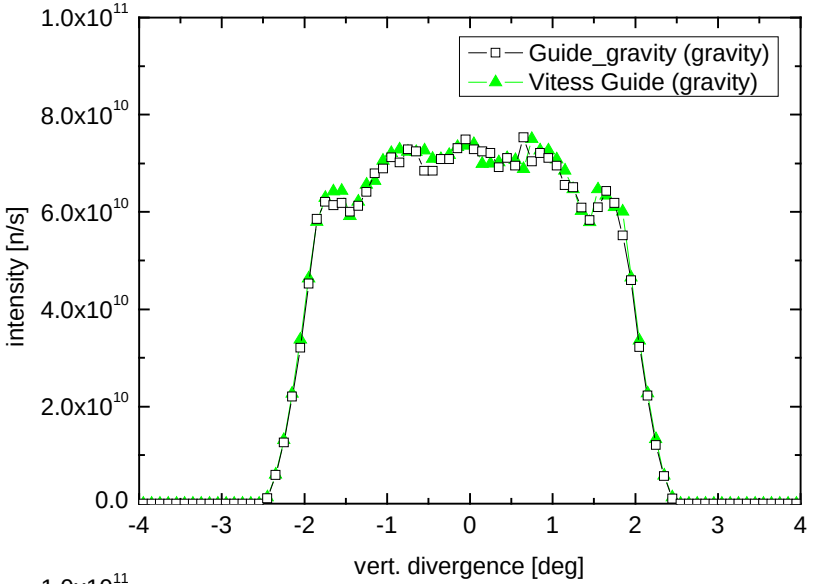
Comparison: count rates at the different parts of the instrument

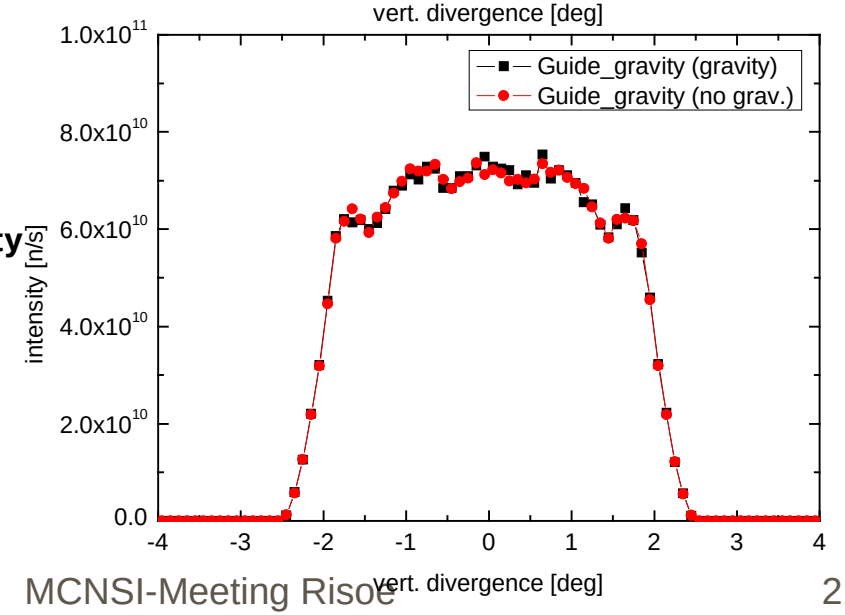
Divergence at exit

Maximal theoretical value: 2.366°



Maximal theoretical value: 2.489°





- Results (after correction of Guide_gravity)
  - **perfect agreement between Guide and Guide_gravity (in the absence of gravitation)**
  - **good agreement between McStas and VITESS simulations (with gravity)**
  - **hardly any effect of gravity**
  - **maximal values correct**

Evaluation and Outlook

- Summary
  - 'Source_gen' : validated (no bug found)
  - 'Guide' : validated (no bug found)
  - 'Guide gravity' : validated (no problems left)
  - 'Guide_curved' : not carefully checked yet
    (seems to work fine, but needs additional features)
  - 'Selector' : validated (one minor bug corrected)
    option to change sense of blade curvature should be added
  - 'V-selector' : validated (no bug found)
    origin of coordinate system should be moved)
- Already checked before
  - Fermi choppers
- To be checked next to have a set of components sufficient to simulate a 'normal' neutron scattering instrument:
  - 'monochromators'
  - 'Chopper'
  - 'Monitor_nD'

Acknowledgement

- Thanks for support, preliminary work, report of bugs, ... to
  - Martin Böhm
  - Heloisa Bordallo
  - Emmanuel Farhi
  - Thilo Seydel
  - ...

References:

R. Peacock et al., internal report at ILL

M. Marseguerra, G. Pauli, Nucl. Instr. Meth. 4 (1959) 140-150.

J. Peters, Nucl. Instr. Meth. Phys. Res. (2005)

Thank you for your attention !

This research project has been supported by the European Commission under the 6th Framework Programme through the Key Action: Strengthening the European Research Area, Research Infrastructures. Contract n°: RII3-CT-2003-505925