

# New release of RESTRAX, ver. 4.8

J. Šaroun<sup>1</sup>, J. Kulda<sup>2</sup>, V. Ryukhtin<sup>1</sup>

<sup>1</sup>*Nuclear Physics Institute, Řež*

<sup>2</sup>*Institute Laue-Langevin, Grenoble*

## Contents:

- New features in RESTRAX (TAS resolution & data fitting)
- New features in SIMRES (ray-tracing)
- Examples of new components:
  - **virtual cold source** – using TRIPOLI output
  - **lobster-eye guides** – comparison with focusing monochromator
- Discussion – MCNSI milestones

see <http://omega.ujf.cas.cz/restrax/>

# New release of RESTRAX, ver. 4.8

## New in RESTRAX 4.8.1:

### sample “exchanger” (EXCI)

Using **runtime modules** to describe scattering at the sample permits to fit/simulate data for different models without restart.

Problems in FORTRAN – solved by C-wrapper calling *dlopen* ...

### simulated data (GENDT)

Generates data incl. counting statistics, using  $S(\mathbf{Q}, \omega)$  from a runtime module.

Permits **virtual experiments**.

### improved job-files

Extended syntax of job files permits to create guided sessions: **tutorials**

4 examples in RESTRAX and 3 in SIMRES are available in the current release

### 3-column data format

data in a simple format [x,y,error] can be loaded (e.g. pre-processed by *Mview*)

# New release of RESTRAX, ver. 4.8

## **RESTRAX documentation:**

### **source documentation**

*html* pages of source code with cross-references is generated by *perl* script (derived from *for2html*) [see here](#)

### **manual to RESTRAX**

The manual is published at the RESTRAX homepage (both html & PDF) [see here](#)

### **mailing list**

Information on program updates/patches will be sent, visit RESTRAX homepage for subscription

# New release of RESTRAX, ver. 4.8

## New in SIMRES 5.0.1:

### features from RESTRAX

command line interface, installation scripts, source docs, *etc.*

### parabolic & elliptic guides

Functionality of the collimator component has been extended :

- slit / channel
- Soller collimator (optionally convergent, oscillating)
- neutron guide or bender
- **guide with parabolic or elliptic profile**
- **lobster-eye guide** (1 or 2 dimensional), with straight, parabolic or elliptic lamellae

### virtual source with inhomogeneous flux distribution

rectangular or circular area using 1- and 2-dimensional look-up tables

table for H53 generated by resampling the output of TRIPOLI (by G. Campioni)

# Virtual cold source

**Inhomogeneous source:**  $\frac{\partial}{\partial \lambda} \phi(x, y, k_x, k_y, \lambda)$

**A.** Using output of core simulations (e.g. from TRIPOLI):

**too low events density** for propagation behind monochromator

$d\Omega \sim 0.0003$ ,  $\Delta\lambda/\lambda \sim 0.01$

**=> only 500 neutrons in 1GB file ( $10^7$  events)!**

**B.** Look-up tables : 5-dimensions !

*Covariance matrix from TRIPOLI data:*

	x	y	$k_x$	$k_y$	E
x	1.00				
y	0.00	1.00			
$k_x$	0.28	0.00	1.00		
$k_y$	0.00	0.52	0.00	1.00	
E	0.00	0.00	0.02	-0.03	1.00

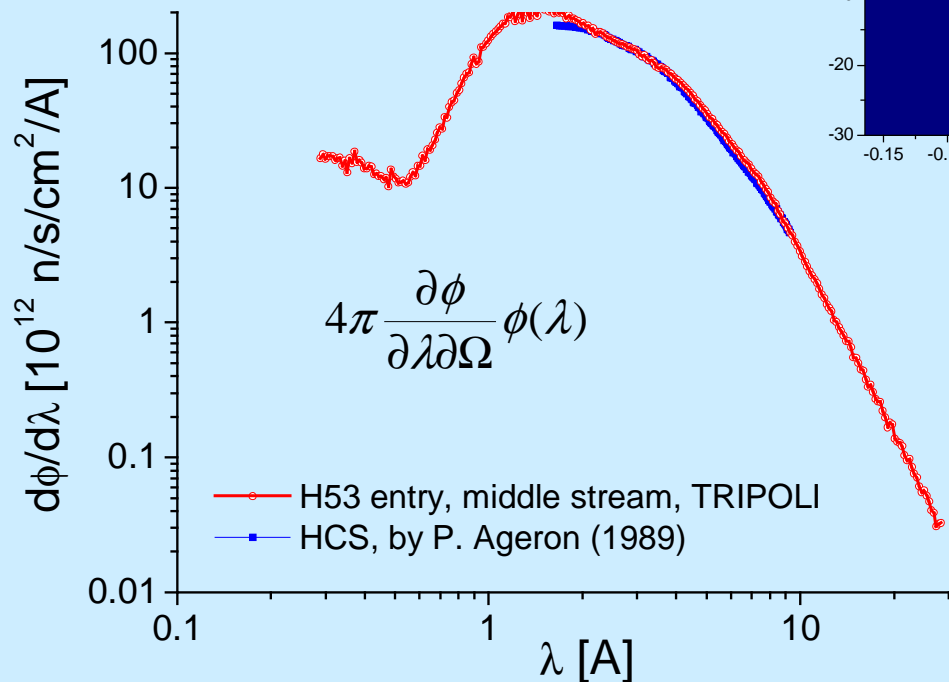
**=> factorisation:**

$$\phi(x, y, k_x, k_y, \lambda) \cong P_H(x, k_x) P_V(y, k_y) \phi_\lambda(\lambda)$$

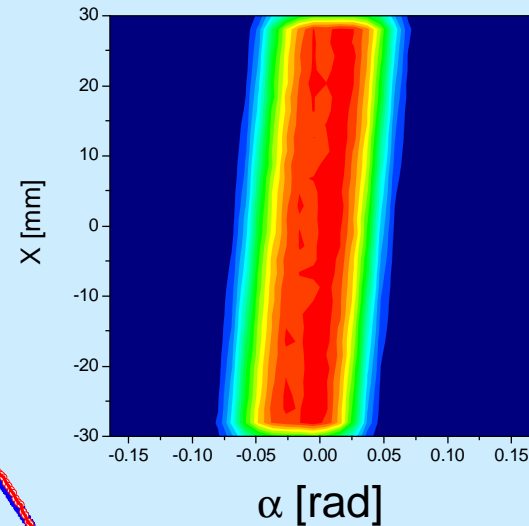
# Virtual cold source

Resampling TRIPOLI data for H53:

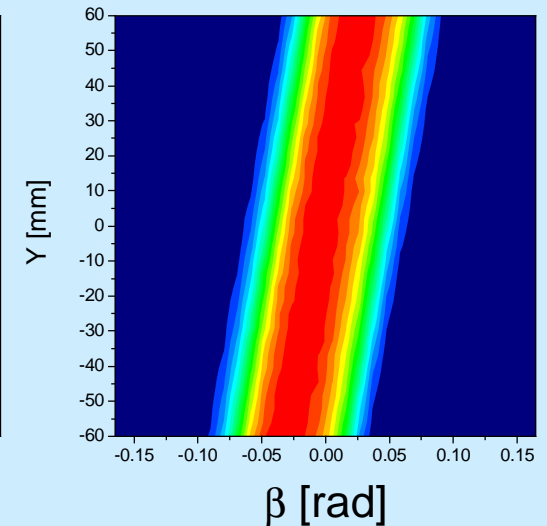
in the middle stream



*horizontal*



*vertical*

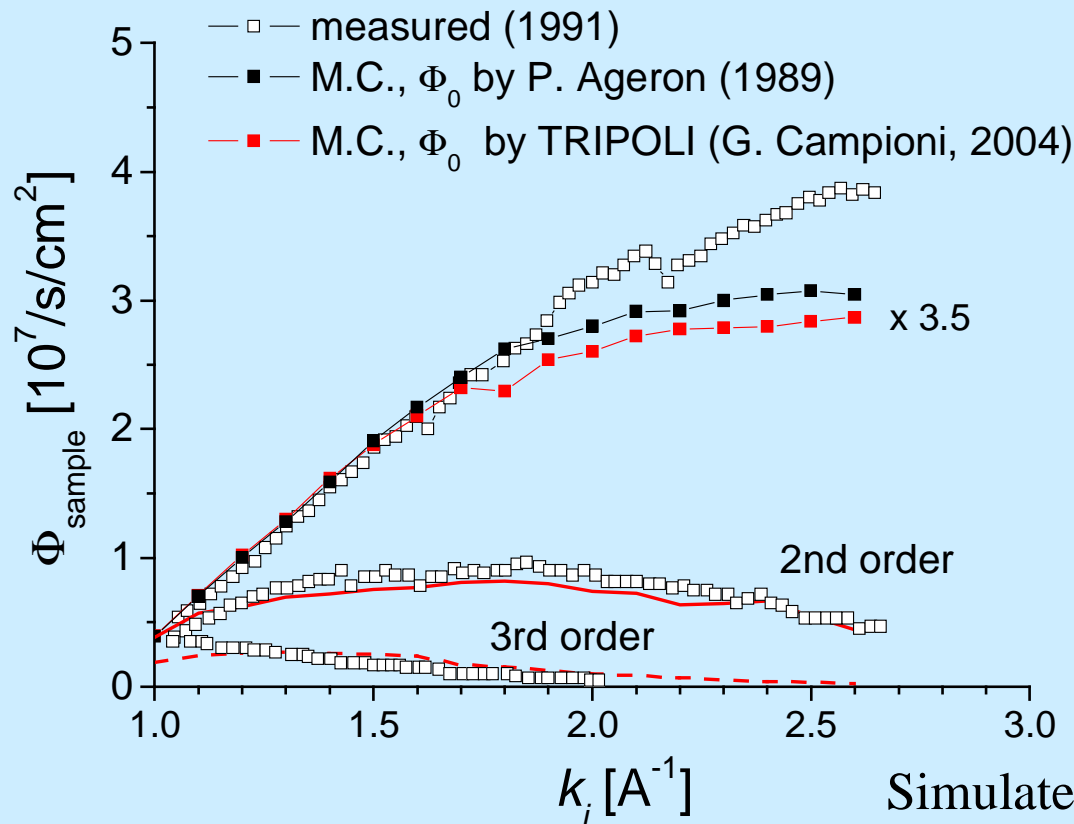


used as look-up tables  
in RESTRAX  $\Rightarrow$

# Virtual cold source

## Monochromatic flux at the sample for IN14:

PG 00.2,  $\alpha_2=40'$



### Capture flux in H53:

distance	$\phi$ [ $10^{10}$ n/s/cm <sup>2</sup> ]
0.0 m	53.0
2.75 m	7.7
9.5 m	4.0
16.4 m	3.7

Simulated flux 3.5 times higher (consistent with McStas results). **Is there a problem with the guide ?**

# Focusing on small samples

Demonstration of new components:

elliptic & parabolic lobster-eye optics

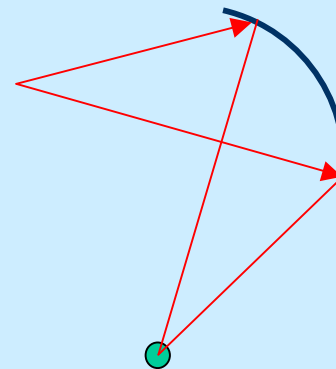
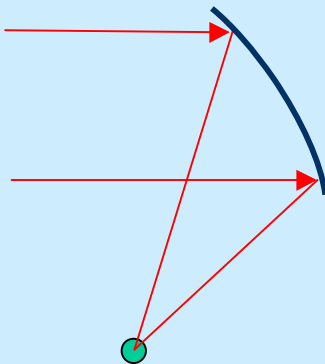


# Focusing on small samples

## A. Focusing crystal array

- Beam size at focal point given by the size of segments
- Simultaneous focusing in space and energy is not possible (with exceptions)

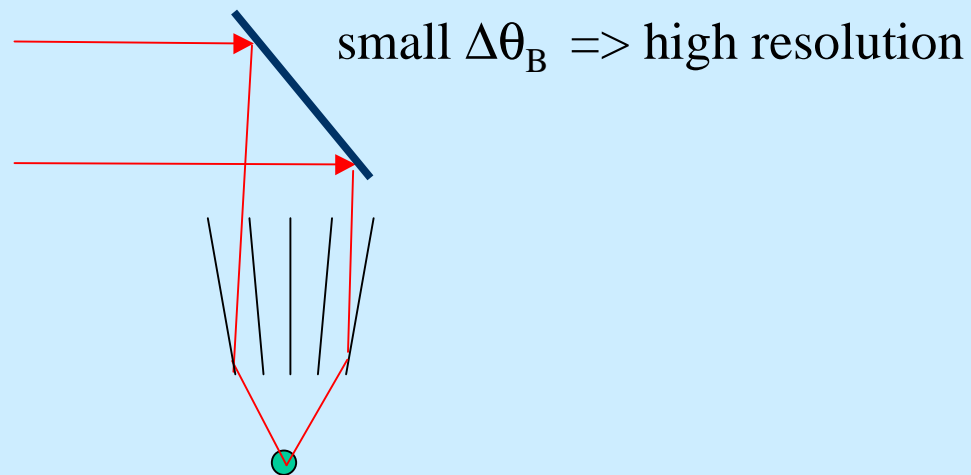
$$f_X = R \sin(\theta_B) \quad ? \quad f_E = 2R \sin(\theta_B)$$



# Focusing on small samples

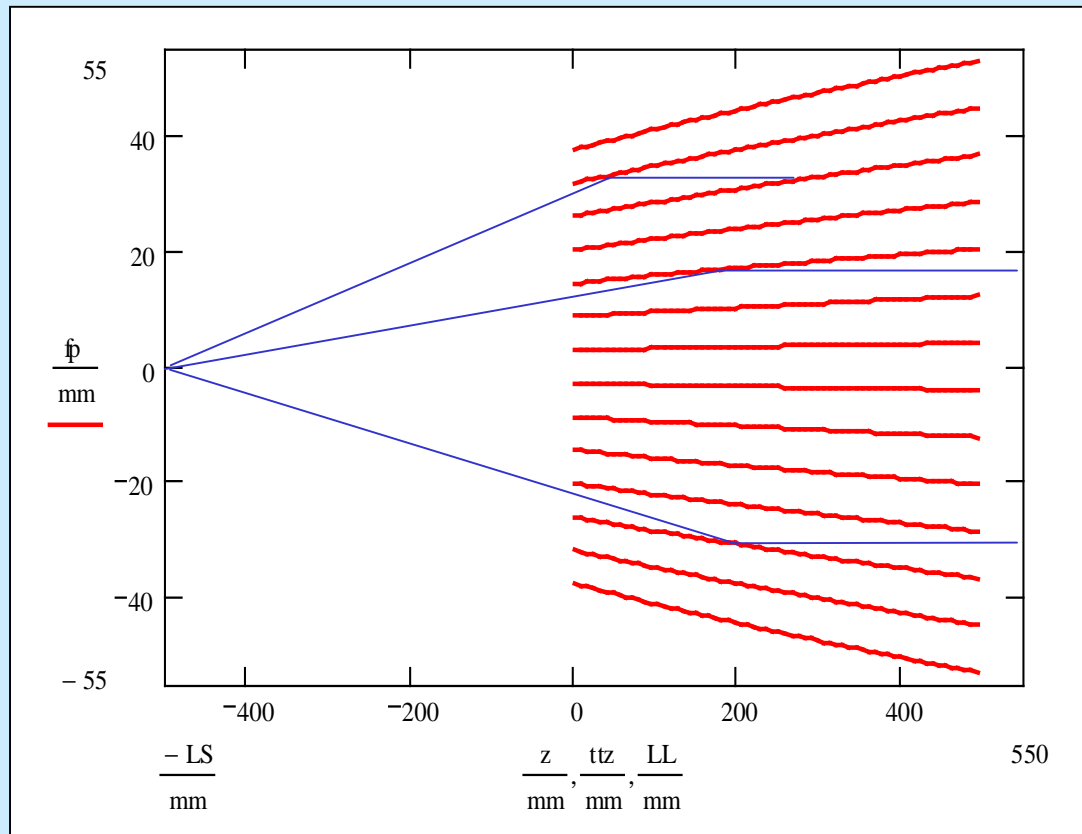
## B. Supermirror optics

- small critical angle
- reflectivity  $< 1$
- minimum distance from the sample is required



# Focusing on small samples

## Parabolic guide

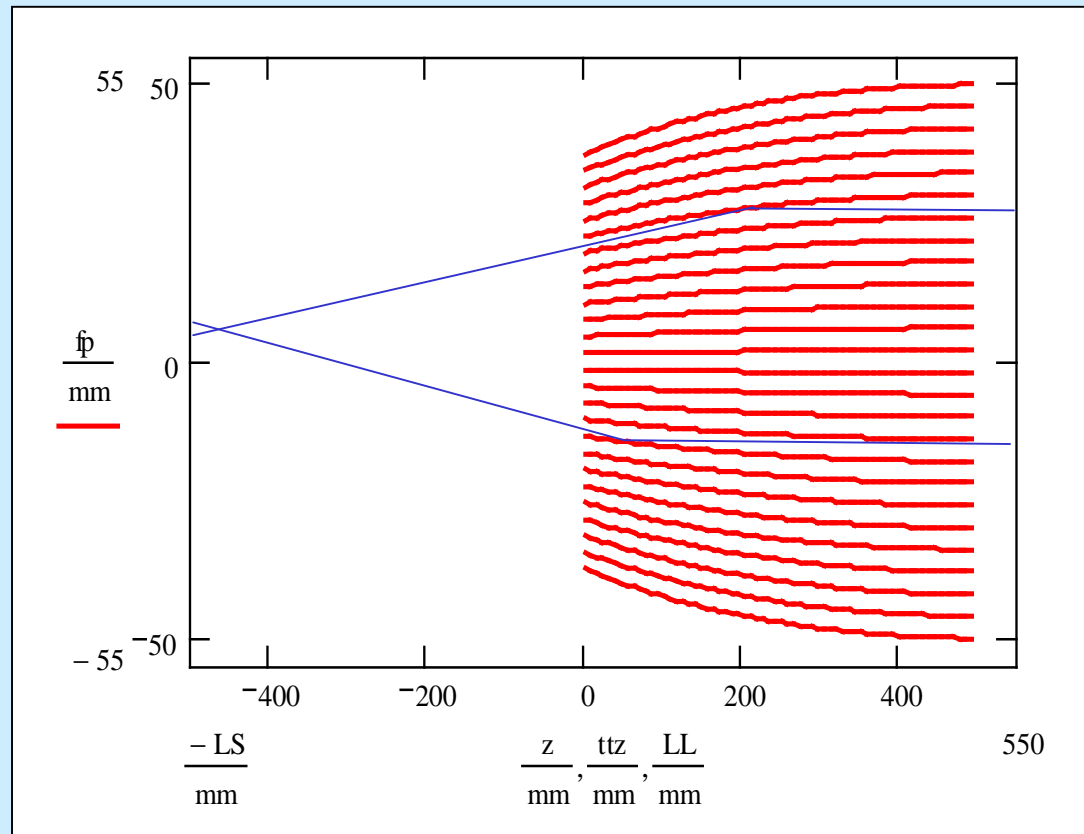


+ perfect focusing of a parallel beam

- large reflection angle at the entry

# Focusing on small samples

## Elliptic guide



- parallel beam does not focus to a point

- lamellae are parallel at the entry

# Focusing on small samples

## **Simulations for the cold neutrons TAS – IN14**

cold source (using TRIPOLI data),  $k_i=1.55 \text{ \AA}^{-1}$

16.4 m straight guide (m=Ni58),  $6 \times 12 \text{ cm}^2$

...

### **with some modifications:**

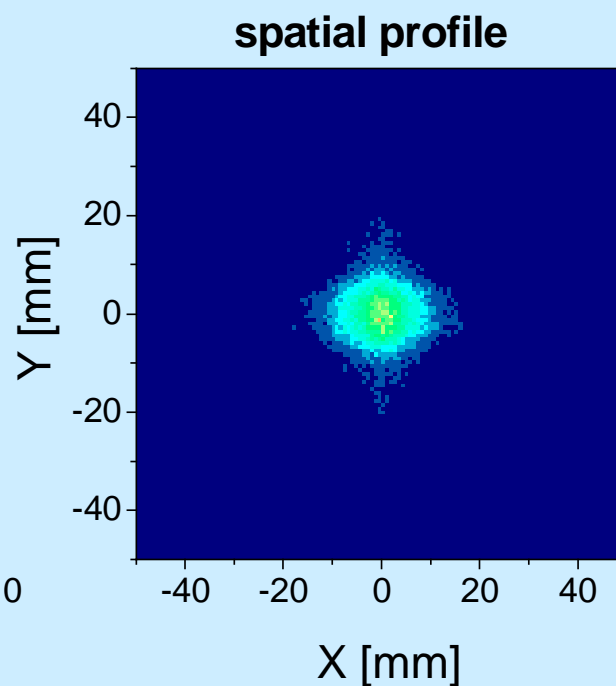
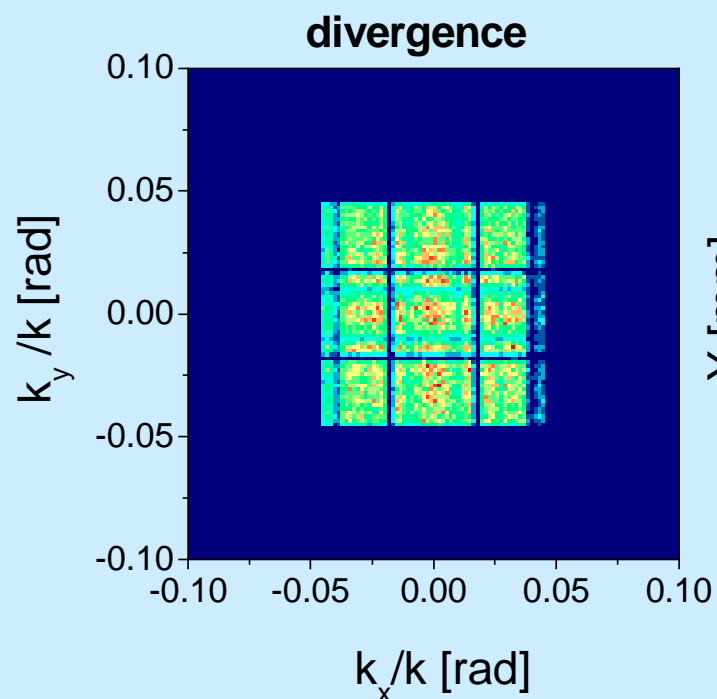
- doubly focusing PG monochromator (7x9 segments)
- shorter sample distance (2.1 m)
- lobster-eye guide:
  - length = 50 cm**
  - distance from the sample = 50 cm**
  - entry area = 10 x 10 cm<sup>2</sup>**

**setup optimizations:** maximum flux at  $1 \times 1 \text{ mm}^2$  sample area

- crystal curvatures (numerically with ray-tracing)
- exit area

# Focusing on small samples

## Parabolic guide, flat monochromator



### Optimized parameters:

number of lamellae: 13 x 13

exit area: 7.0 x 7.0 cm<sup>2</sup>

### Results:

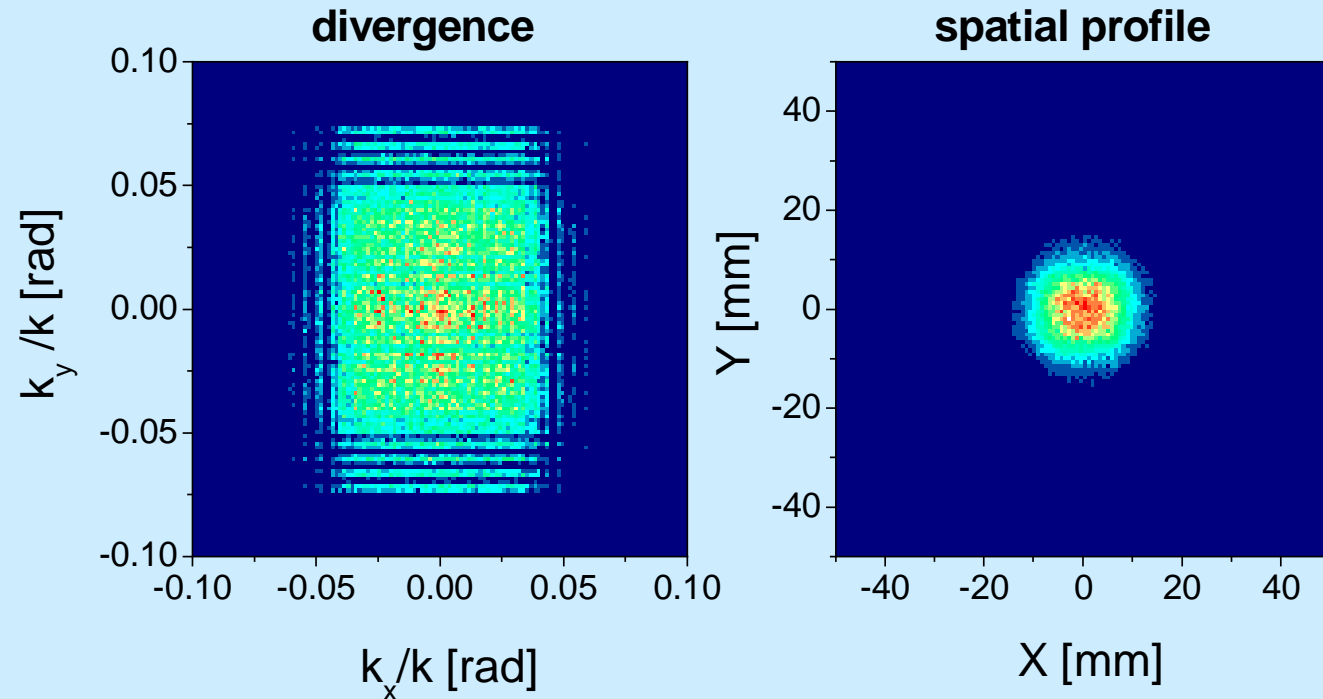
flux [10<sup>6</sup>/s/mm<sup>2</sup>] : 7.59

total [10<sup>8</sup>/s] : 17.4

$\Delta E_i$  [meV] : 0.094

# Focusing on small samples

## Elliptic guide, flat monochromator



### Optimized parameters:

number of lamellae: 25 x 25

exit area: 7.3 x 7.3 cm<sup>2</sup>

### Results:

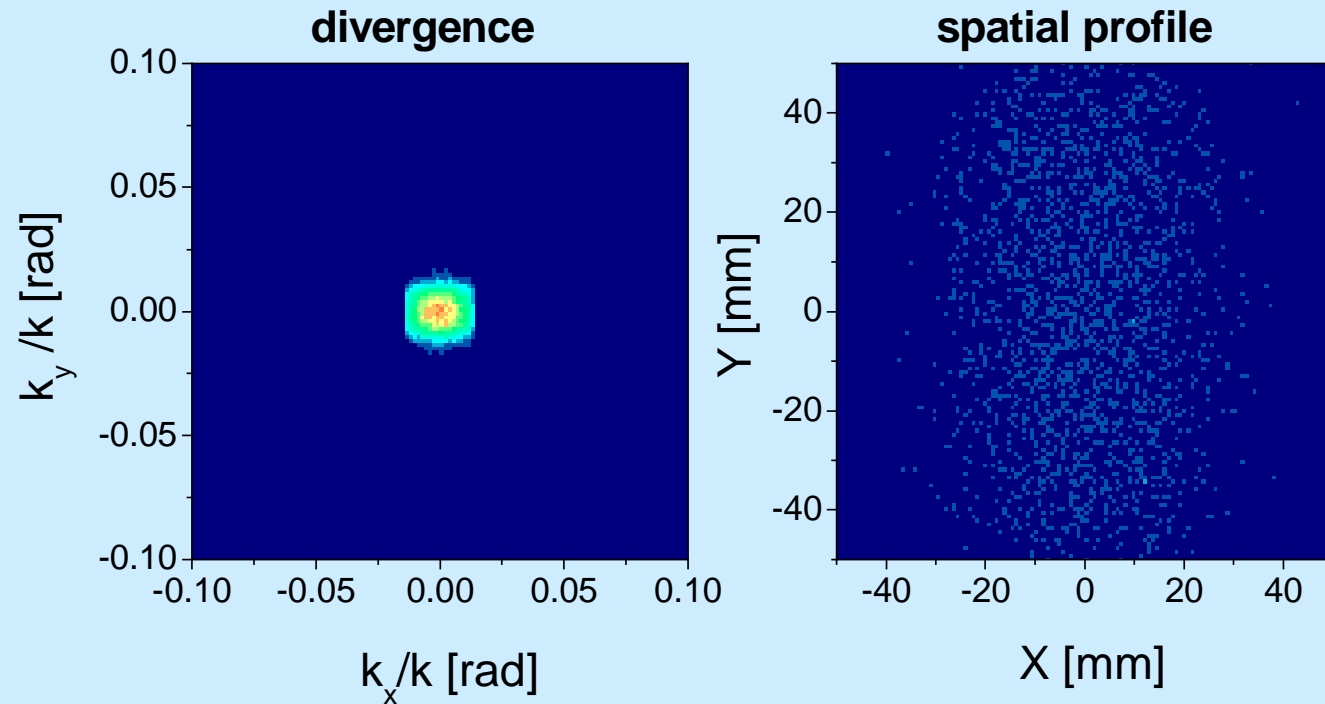
flux [10<sup>6</sup>/s/mm<sup>2</sup>] : 9.74

total [10<sup>8</sup>/s] : 26.2

$\Delta E_i$  [meV] : 0.12

# Focusing on small samples

## No guide, flat monochromator



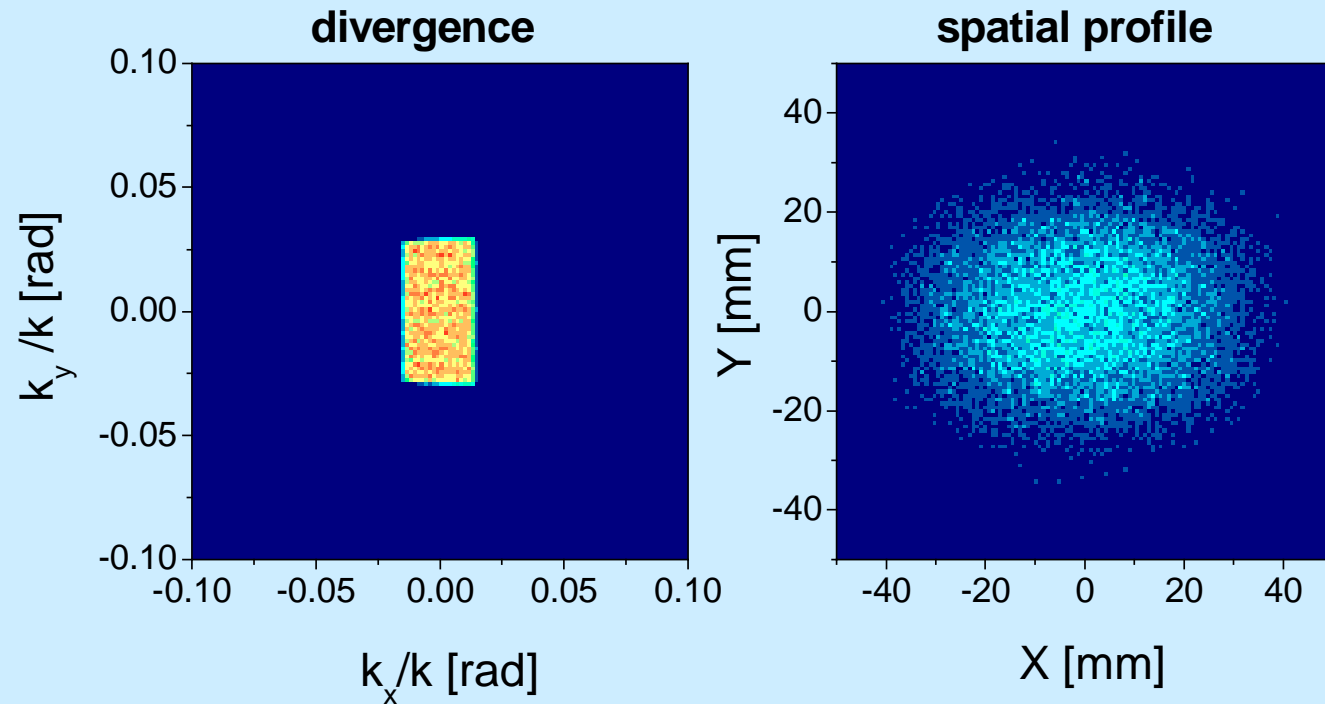
### Results:

flux [ $10^6/s/mm^2$ ] : 0.69  
total [ $10^8/s$ ] : 42.8  
 $\Delta E_i$  [meV] : 0.15



# Focusing on small samples

## No guide, focusing monochromator



### Optimized parameters:

$1/R_H$  [ $m^{-1}$ ]: 0.15

$1/R_V$  [ $m^{-1}$ ]: 0.39

### Results:

flux [ $10^6/s/mm^2$ ] : 2.50

total [ $10^8/s$ ] : 56.7

$\Delta E_i$  [meV] : 0.14

# Focusing on small samples

## Summary

	total	flux	$\Delta E$
parabolic (13 x 13)	1.74E+09	7.59E+06	0.10
elliptic (25 x 25)	2.62E+09	9.74E+06	0.12
no guide	4.28E+09	6.87E+05	0.15
focusing mono	5.67E+09	2.50E+06	0.14

focusing by lobster-eye:

- **gain 4x** in flux compared to focusing by monochromator
- good energy resolution

# MCNSI milestones

## < Q6:

D2.3 first version of RESTRAX manual  
done, + new version release

M2.2 prototype sample components

in RESTRAX: phonons, incommensurate fluctuations, damped oscillators  
SIMRES: powder, Vanad

## < Q8:

D2.4 new release with NeXus format

possible, but needs specification, xml format (DTD for TAS?)

M3.4 common simulation (steady-state)

IN14? (partially done)