# Introduction to RESTRAX

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**Contents:**

- Overview of RESTRAX features
- Example of TAS simulations with flat-cone multianalyzer
- Overview of SIMRES features
- Example: multichannel supermirror guides


RESTRAX homepage: http://omega.ujf.cas.cz/restrax/

# RESTRAX package

## What is RESTRAX?

### Virtual three-axis neutron spectrometer

- Modeling of TAS **resolution functions** using both analytical (matrix) and Monte Carlo ray-tracing methods.
- **4D convolution** with an "arbitrary" scattering kernel – S($\boldsymbol{q}$,$\omega$) function
- **data analysis** (non-linear $\chi^2$ fitting)

## What is SIMRES?

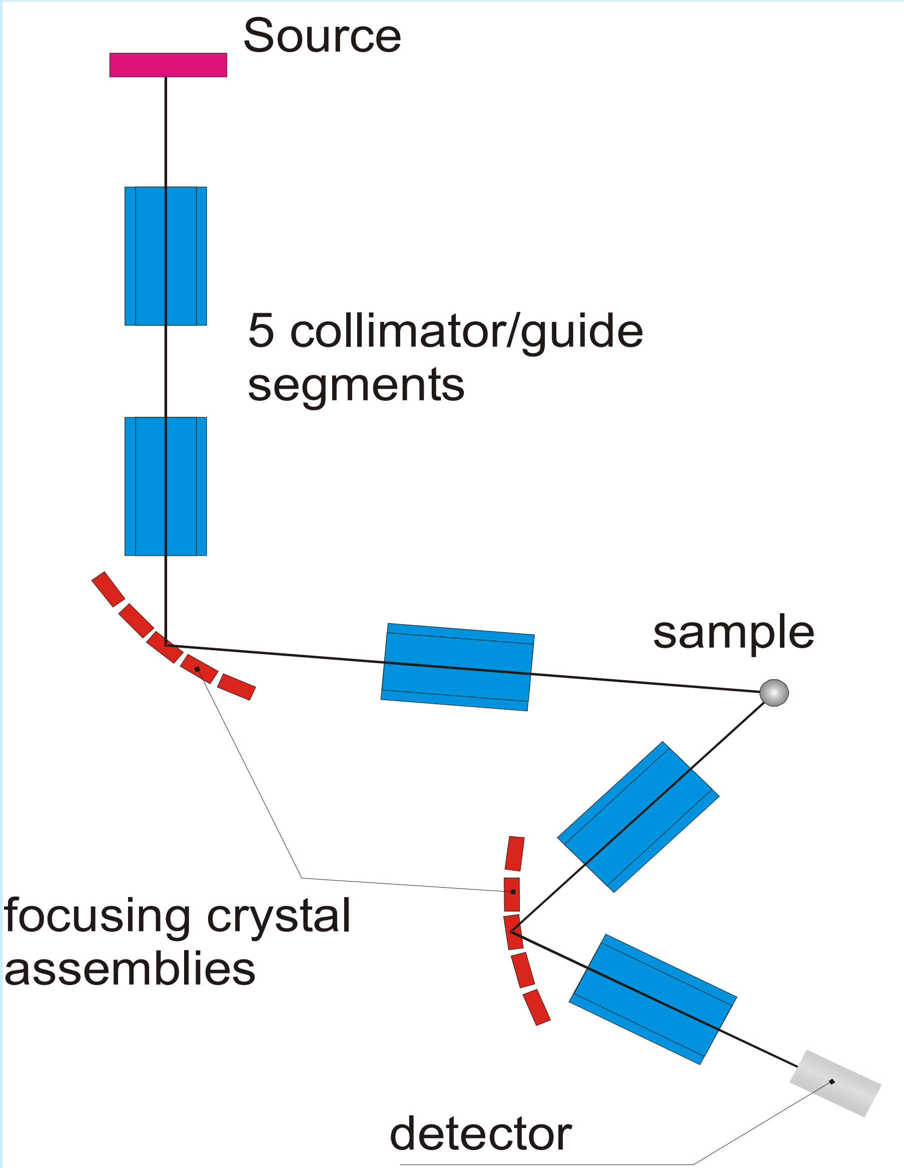
### Ray-tracing simulation program

for instruments with "TAS-like" layout (*e.g.* powder diffractometer)

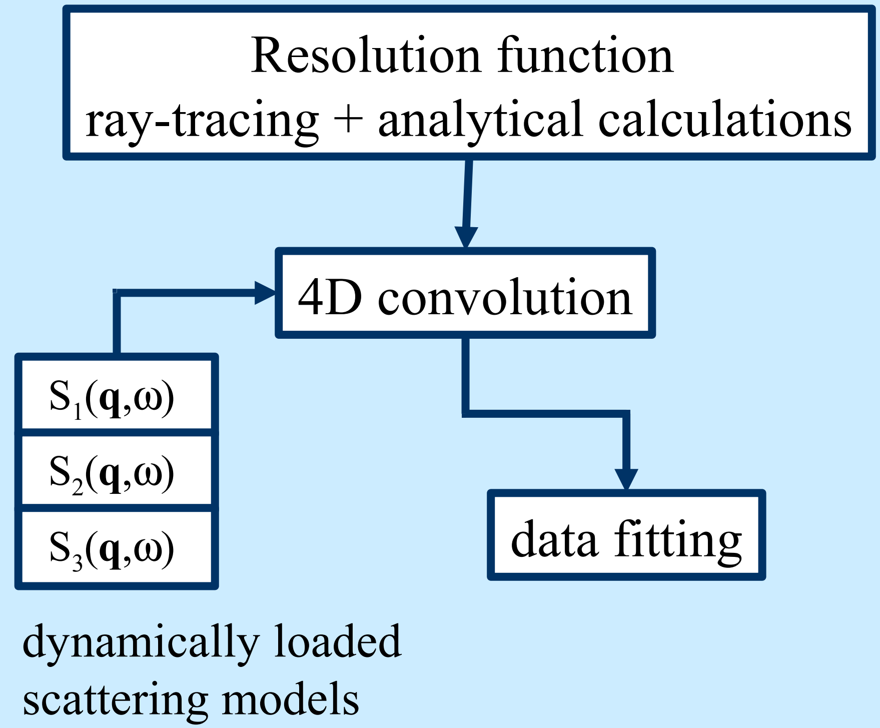
- **More detailed** simulation of some components (benders, crystals)
- Absolute **neutron fluxes and beam profiles** in $\boldsymbol{r}$, $\boldsymbol{k}$, $t$ space.
- **Tools for instrument design** – mapping intensity/resolution in the space of instrument parameters + numerical optimization

Win32 and Linux versions available at http://omega.ujf.cas.cz/restrax

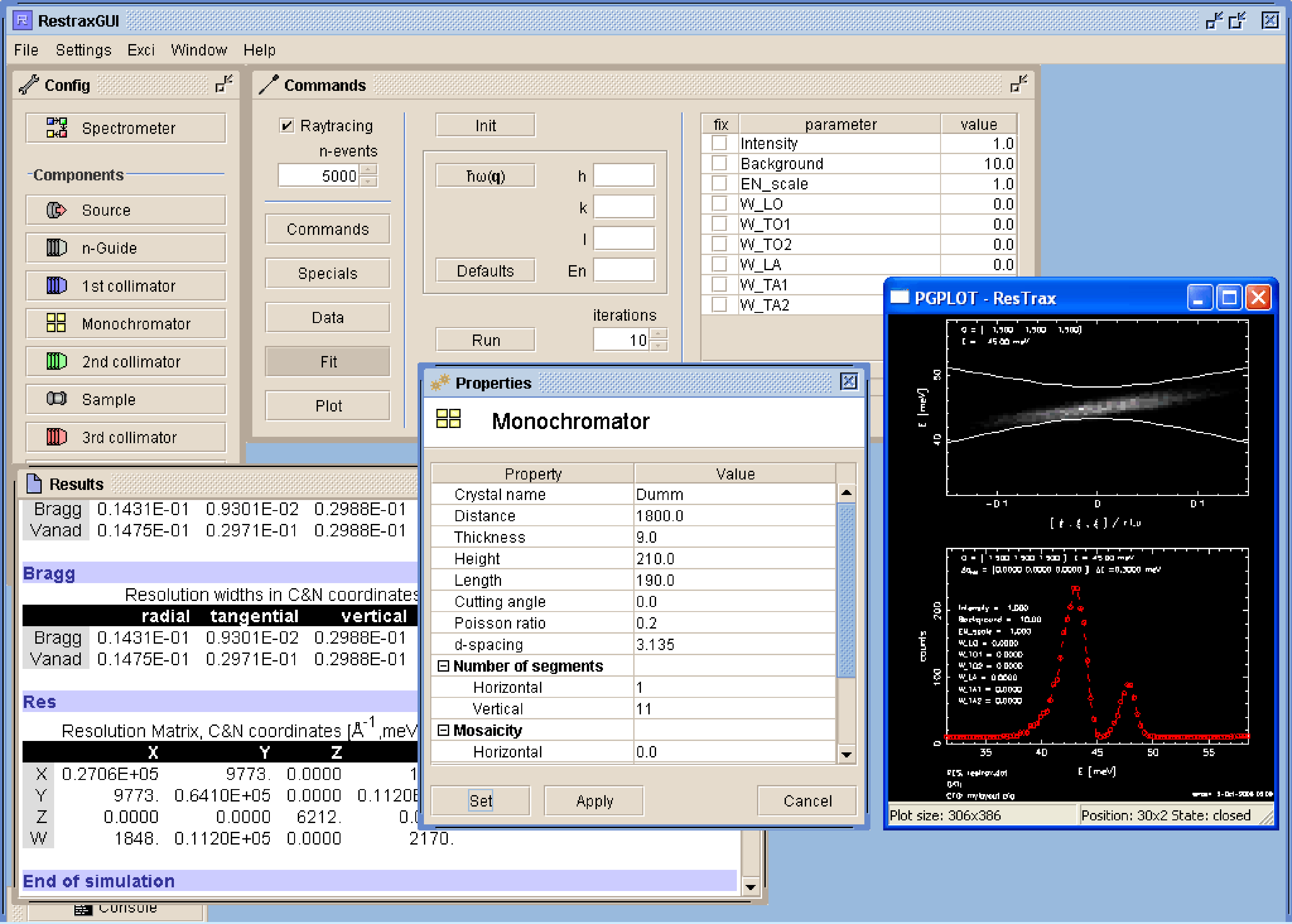
# RESTRAX



Source
5 collimator/guide segments
sample
focusing crystal assemblies
detector

Resolution function
ray-tracing + analytical calculations
4D convolution
$S_1(\mathbf{q},\omega)$
$S_2(\mathbf{q},\omega)$
$S_3(\mathbf{q},\omega)$
data fitting
dynamically loaded scattering models



RestraxGUI
File Settings Exci Window Help
Config
Spectrometer
Components
Source
n-Guide
1st collimator
Monochromator
2nd collimator
Sample
3rd collimator
Commands
Raytracing
n-events
5000
Commands
Specials
Data
Fit
Plot
Init
ħω(q)
h
k
l
Defaults
En
iterations
Run
10
fix
parameter
value
Intensity 1.0
Background 10.0
EN_scale 1.0
W_LO 0.0
W_TO1 0.0
W_TO2 0.0
W_LA 0.0
W_TA1
W_TA2
PGPLOT - ResTrax
Plot size: 306x386
Position: 30x2 State: closed
Properties
Monochromator
Property
Value
Crystal name Dumm
Distance 1800.0
Thickness 9.0
Height 210.0
Length 190.0
Cutting angle 0.0
Poisson ratio 0.2
d-spacing 3.135
Number of segments
Horizontal 1
Vertical 11
Mosaicity
Horizontal 0.0
Set
Apply
Cancel
Results
Bragg 0.1431E-01 0.9301E-02 0.2988E-01
Vanad 0.1475E-01 0.2971E-01 0.2988E-01
Bragg
Resolution widths in C&N coordinates
radial tangential vertical
Bragg 0.1431E-01 0.9301E-02 0.2988E-01
Vanad 0.1475E-01 0.2971E-01 0.2988E-01
Res
Resolution Matrix, C&N coordinates [Å-1,meV
X Y Z
X 0.2706E+05 9773. 0.0000
Y 9773. 0.6410E+05 0.0000 0.1120E
Z 0.0000 0.0000 6212.
W 1848. 0.1120E+05 0.0000 2170.
End of simulation
Console

# Resolution function: $R(Q,\omega)$

Defined as convolution ...

$$I(\mathbf{Q}_0,\omega_0) = \frac{\sigma}{4\pi} N \frac{k_f}{k_i} \int S(\mathbf{Q},\omega) R(\mathbf{Q}_0 - \mathbf{Q}, \omega_0 - \omega)\, d\mathbf{Q}\, d\omega$$

… or neutron transport

$$I(\mathbf{k}_I,\mathbf{k}_F) = \int W(\mathbf{k}_i,\mathbf{k}_f)\Phi_{\mathbf{k}_I}(\mathbf{r},\mathbf{k}_i) P_{\mathbf{k}_F}(\mathbf{r},\mathbf{k}_f)\, d\mathbf{r}\, d\mathbf{k}_i\, d\mathbf{k}_f$$

Scattering probability

Flux distribution at the sample

Detection probability

# Resolution function obtained by ray-tracing

A "specimen" scattering to all $\boldsymbol{k}_{\mathrm{f}}$ with equal probability:

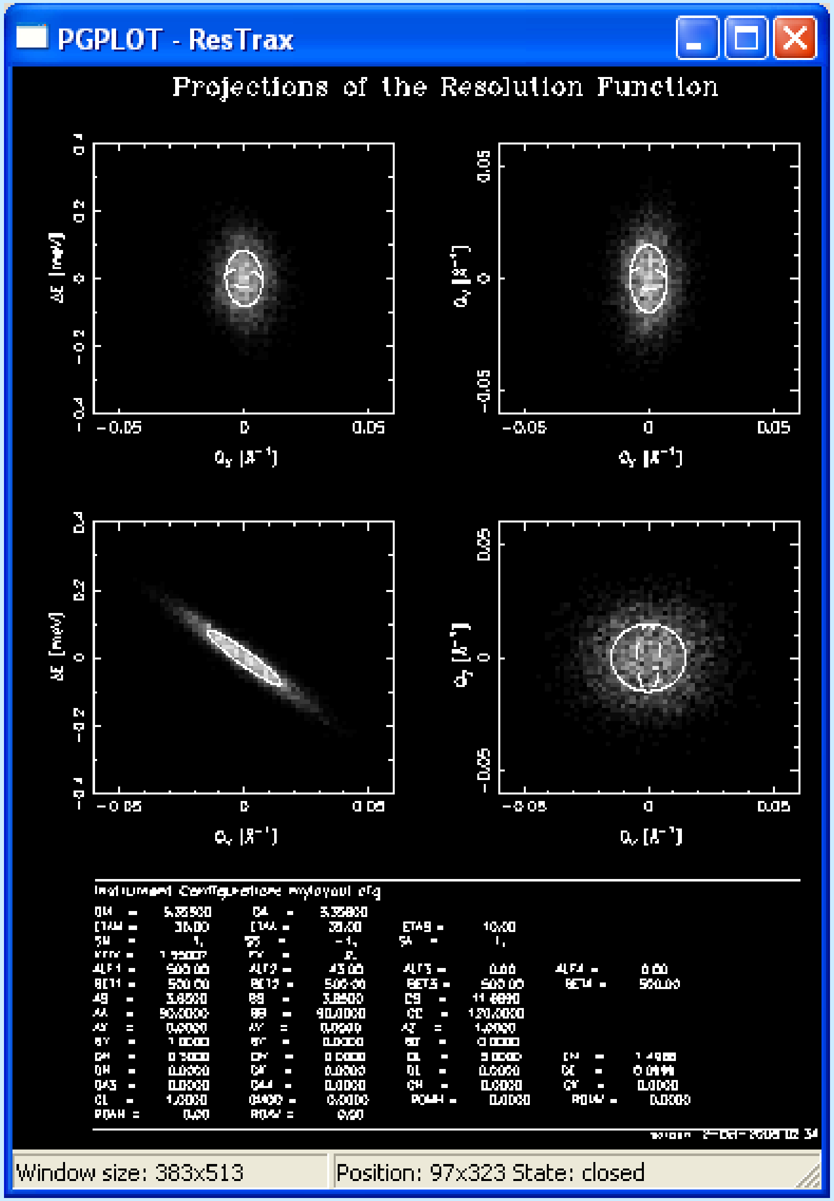
$$E_0 \equiv \frac{\hbar^2}{2m}\left(\left|\mathbf{k}_{i,\alpha}\right|^2 - \left|\mathbf{k}_{f,\alpha}\right|^2\right)$$

$$\mathbf{Q}_\alpha \equiv \mathbf{k}_{f,\alpha} - \mathbf{k}_{i,\alpha}$$

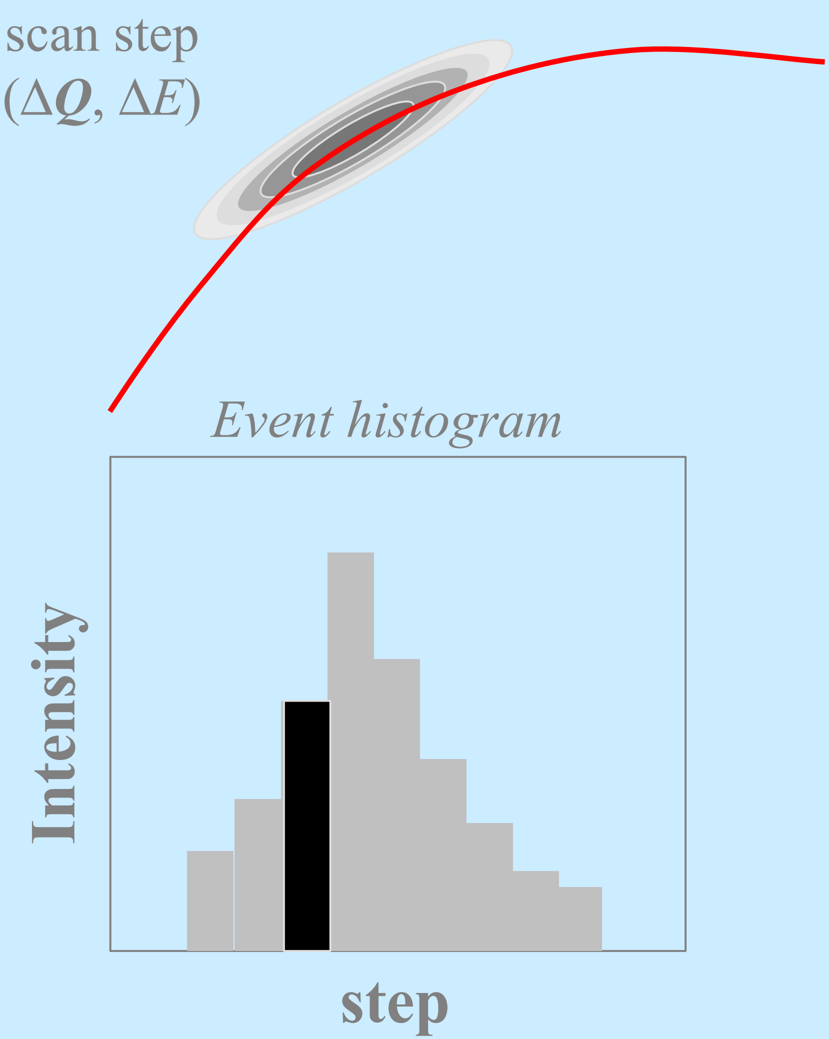
Resolution function is represented by a cloud of points

$$\boldsymbol{X}_\alpha \equiv \left(\boldsymbol{Q}_\alpha, E_\alpha, \ldots\right)$$

weighted by event probability, $p_\alpha$



# Monte Carlo convolution with S(*Q*,*E*)

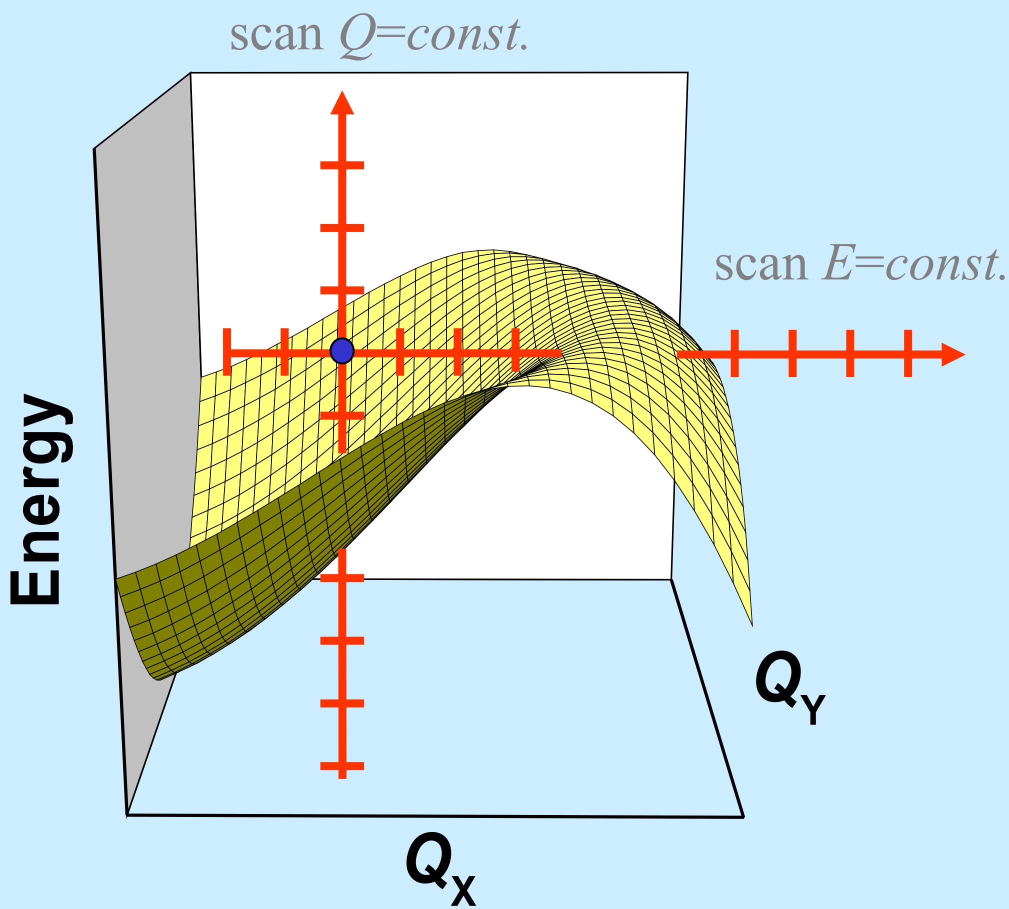



## **Diffuse *S*(*Q*,ω)**

All events are counted at each step:

$$I_j = \sum_{\alpha} p_\alpha S(\mathbf{Q}_\alpha + j\Delta\mathbf{Q}, E_\alpha + j\Delta E)$$

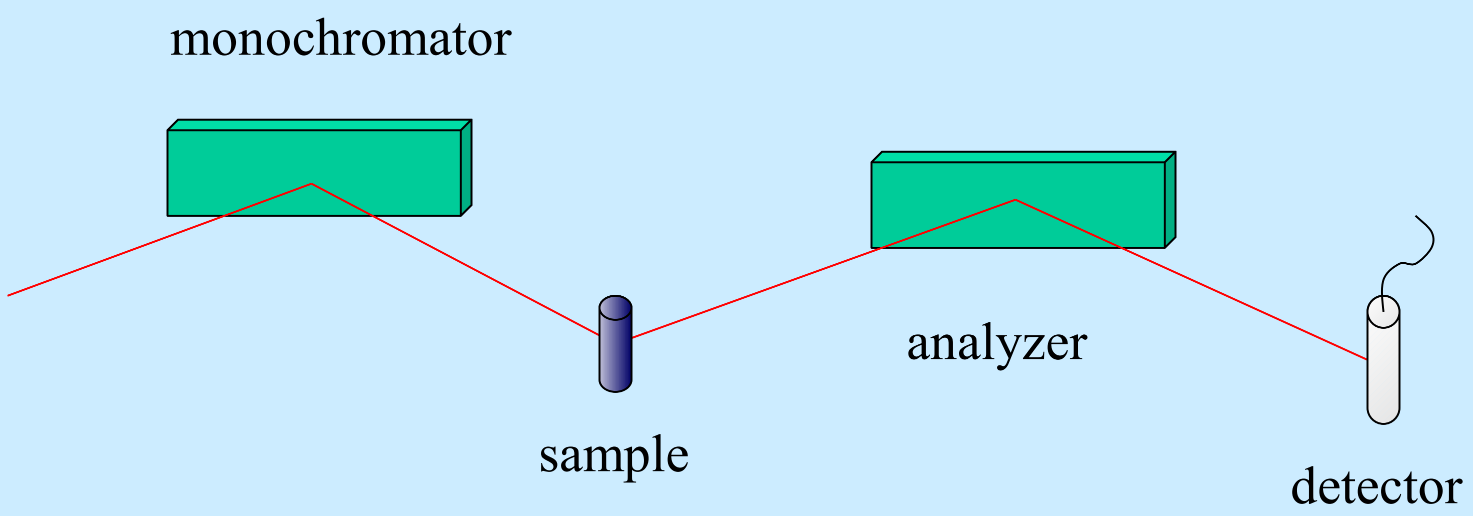
# Monte Carlo convolution with S($\boldsymbol{Q}$,$E$)



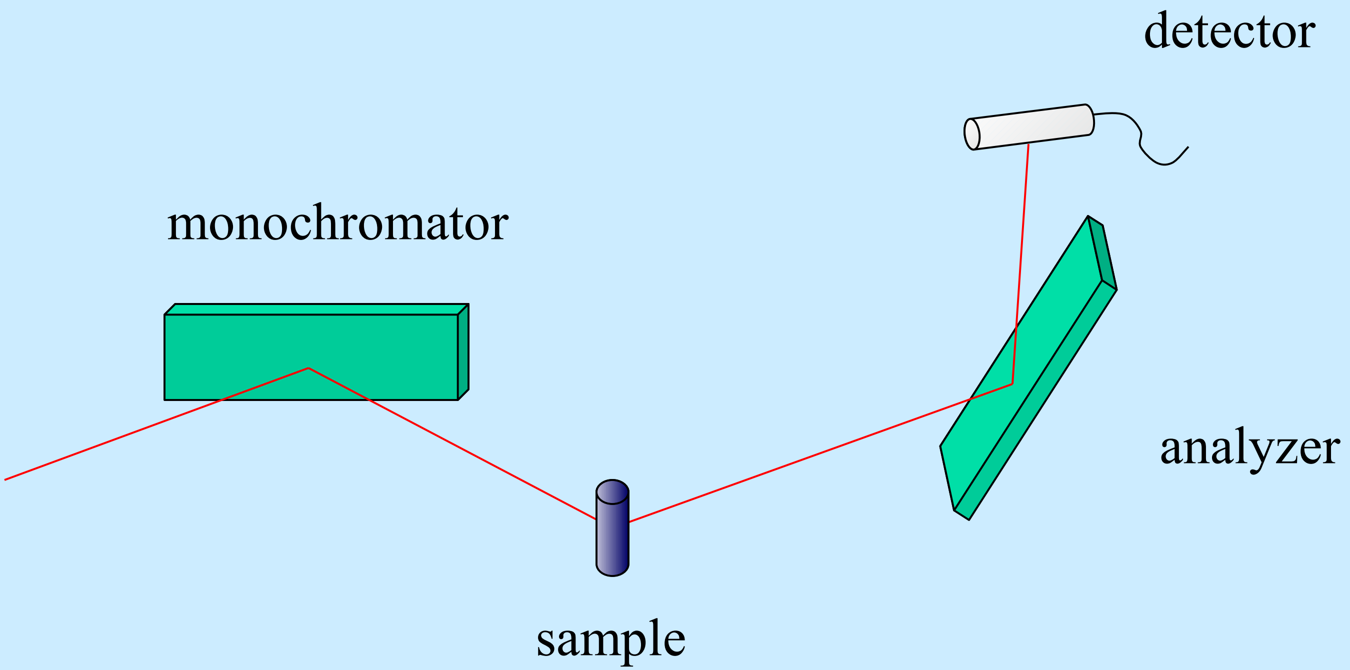

**Zero-width dispersion:**

Events are sorted according to their distance from the dispersion branch

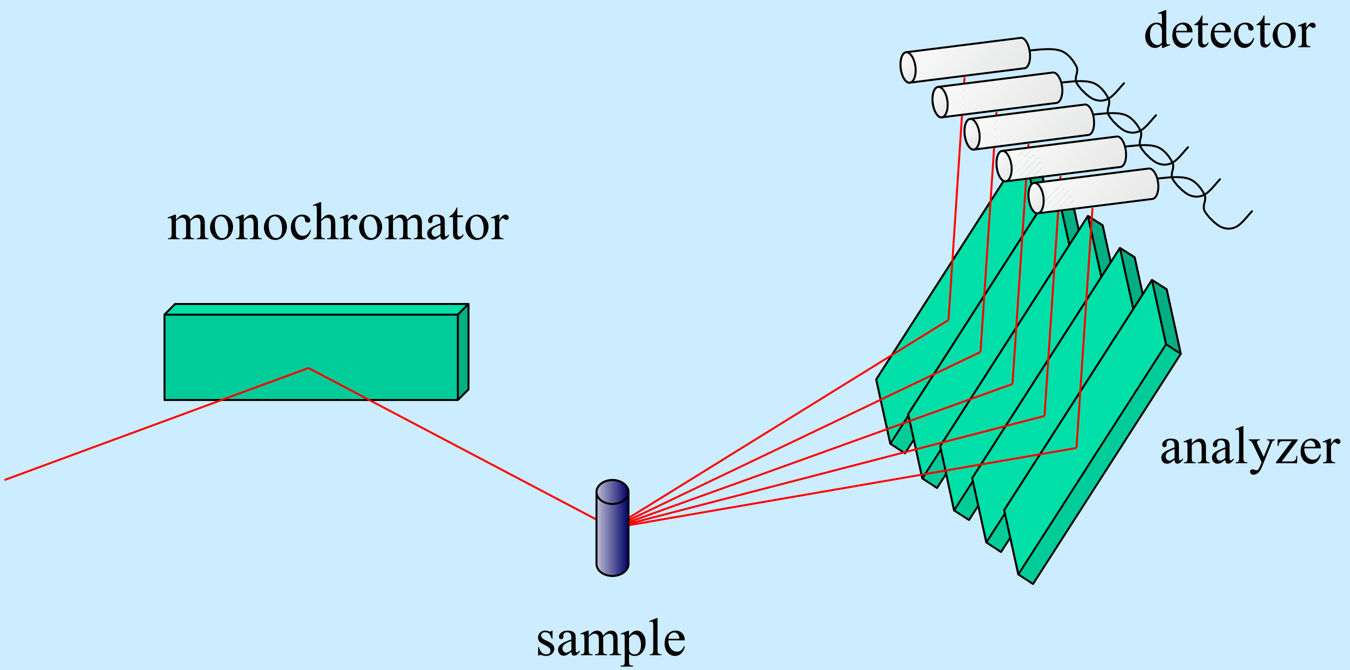
# TAS: conventional arrangement



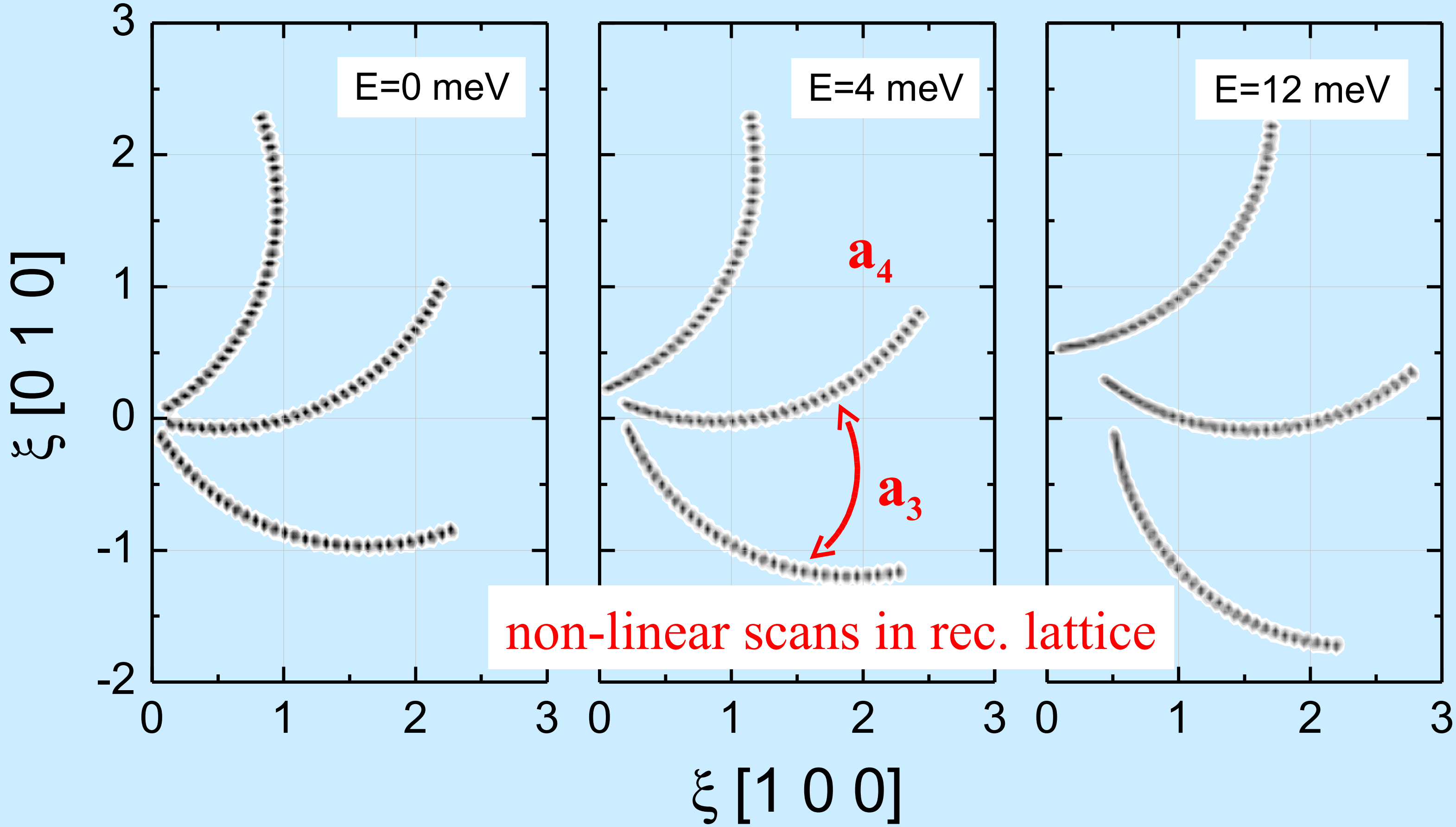
# TAS: flat-cone analyzer



# TAS: flat-cone multianalyzer



# Mapping reciprocal space

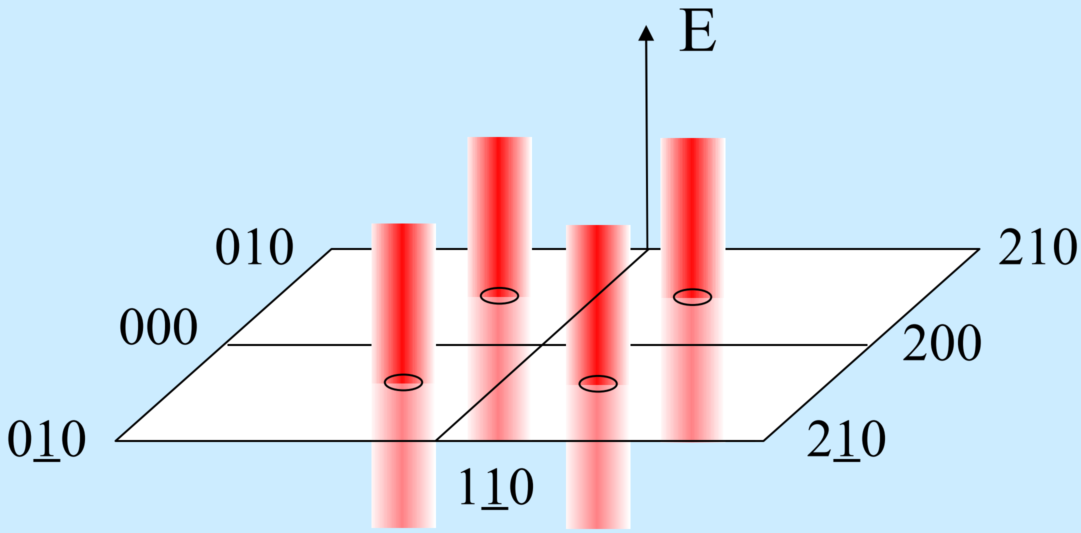



*New flat-cone analyzer for ILL TAS instruments, 32 channels*

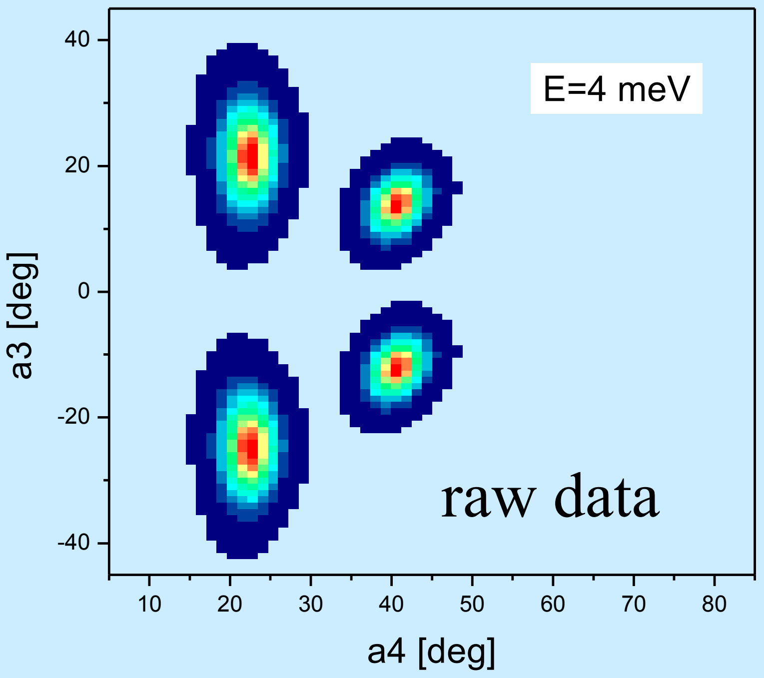
**IN20:** monochromator Si, $k_i$=3 $A^{-1}$

# Example 1: Incommensurate satellites

**Incommensurate satellites**: ΔE →∞

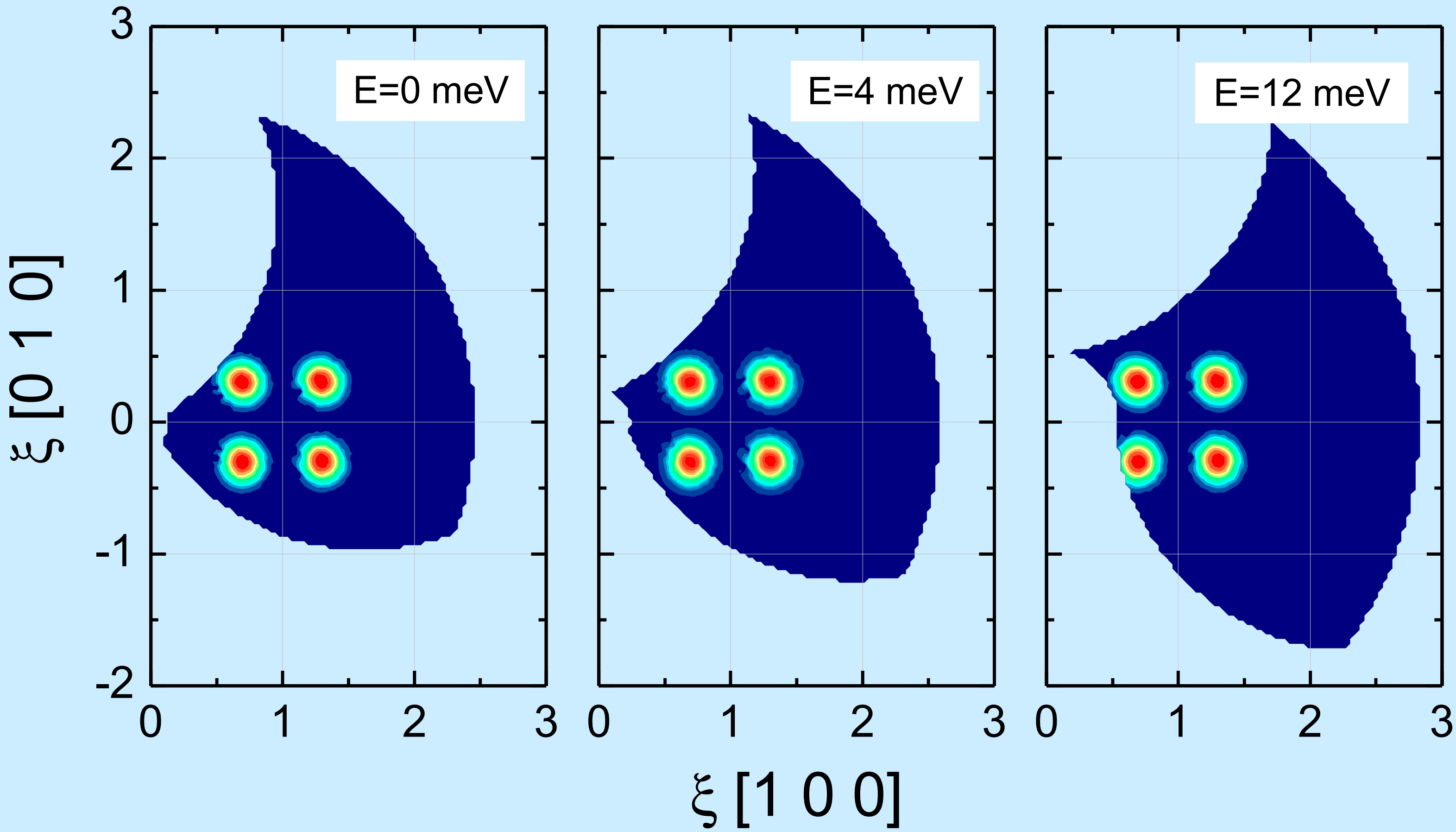



M.C. ray-tracing & convolution with S(*Q*,*E*)



# Example 1: Incommensurate satellites

*… and transformed to rec. lattice space*

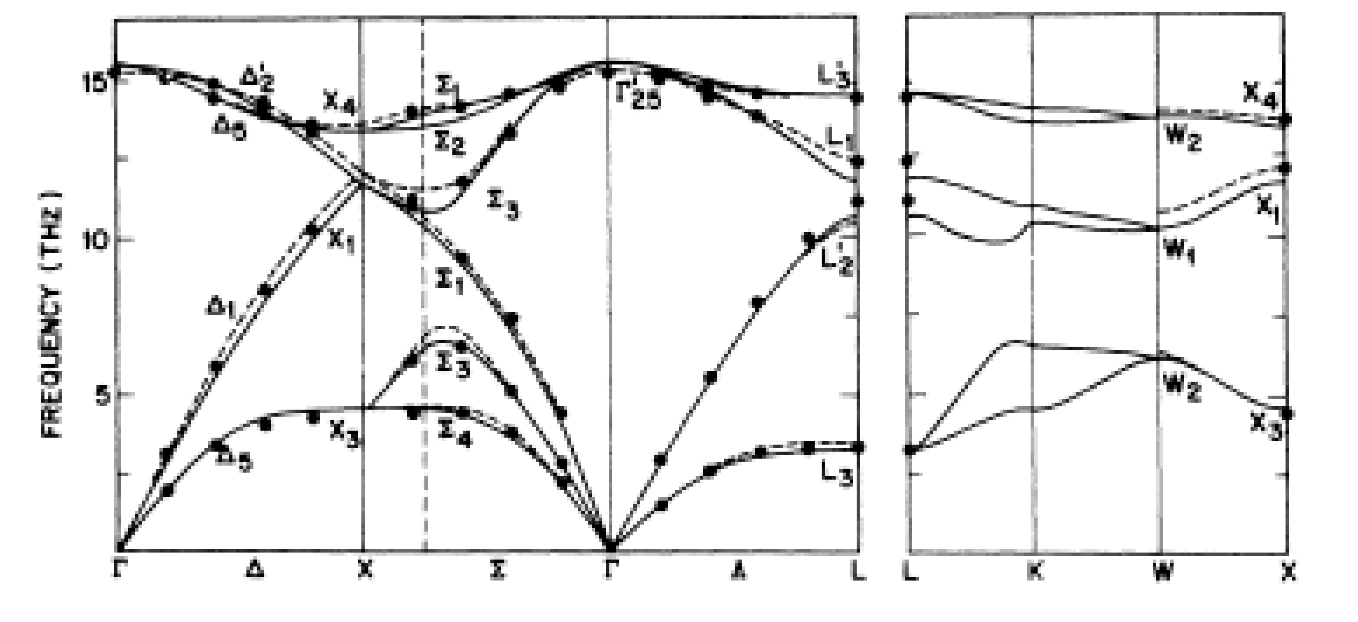


# Example 2: *bond charge model (BCM)*

Model describing ***phonons in diamond lattice*** (Si, Ge, α-Sn, ...)

***Eigenvalues & eigenvectors*** are calculated using ***coulombic potential of bond charges*** for each of *Q,E* points representing simulated TAS resolution function

W. Weber, Phys. Rev. B 15 (1977) 4789.




phonons in Si

# Phonons in Si

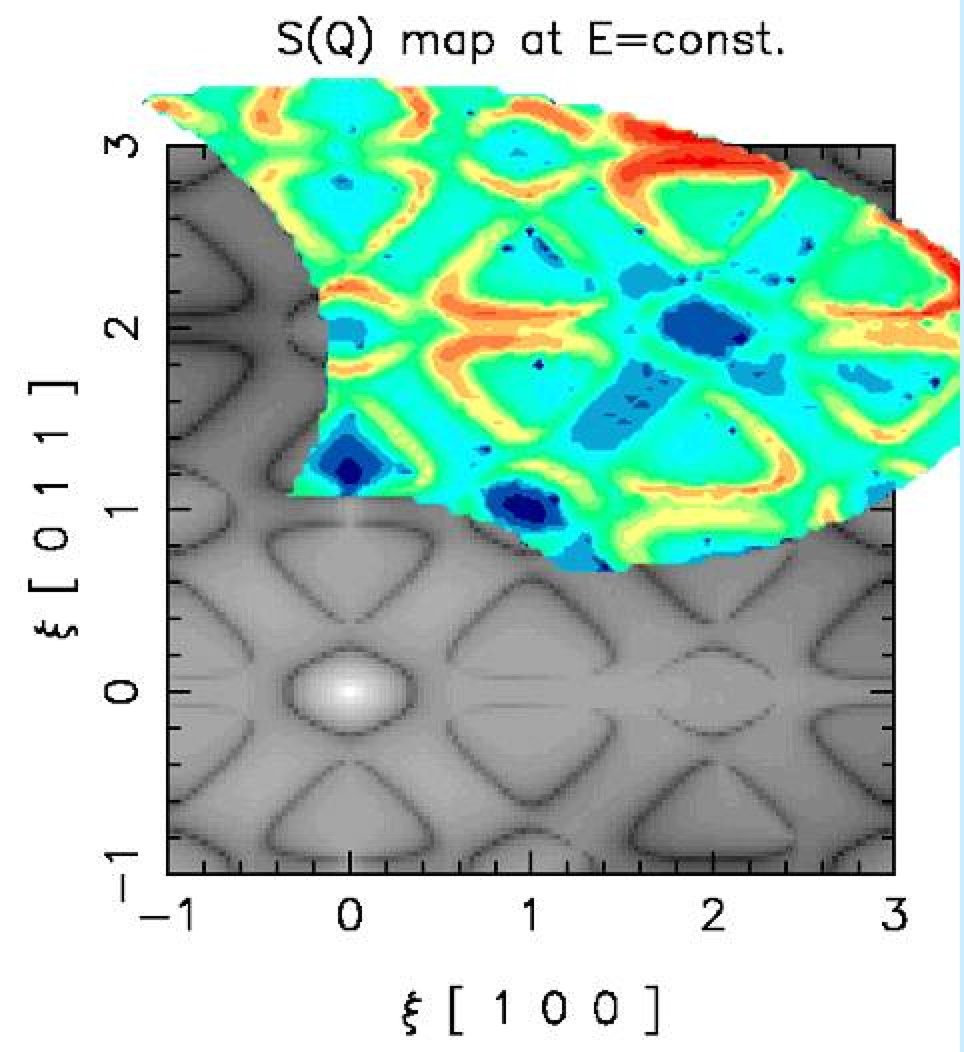
**MC simulation for IN20**

$k_f$=3A$^{-1}$, $E$=20meV

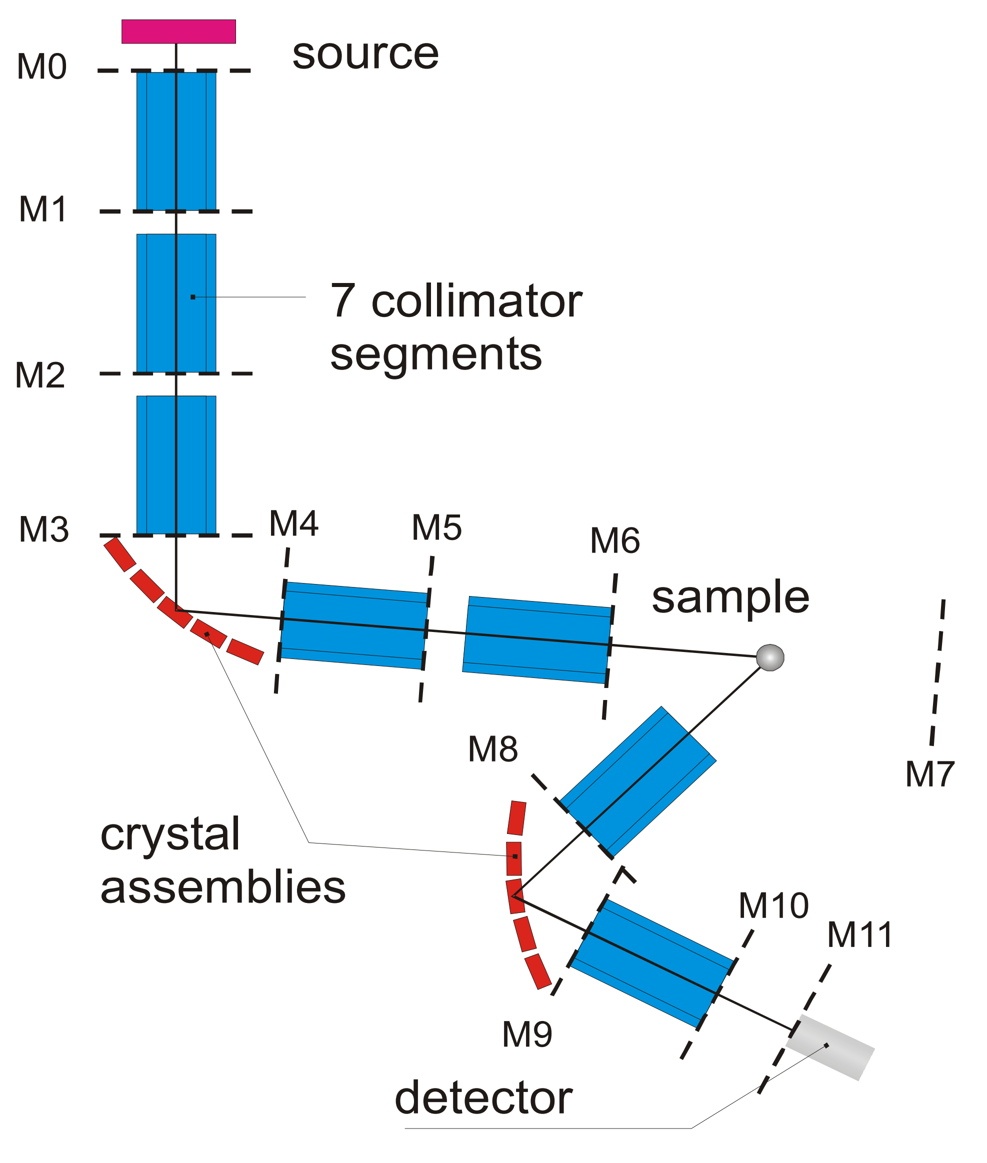
64 channels, Δa4=1.25°

91 steps, Δa3=0.75°

*convolution with flat-cone resolution*
*simulated by ray-tracing*
*CPU time: 4 hours*



# SIMRES




**source:** arbitrary energy, spatial and angular distributions via look-up tables

**crystals:** focusing arrays of elastically bent or mosaic crystals (incl. simulated extinction effects, absorption, etc...)

**collimators:** universal components

- coarse and Soller collimators
- curved guides or benders
- elliptic or parabolic guides (multilamellar)

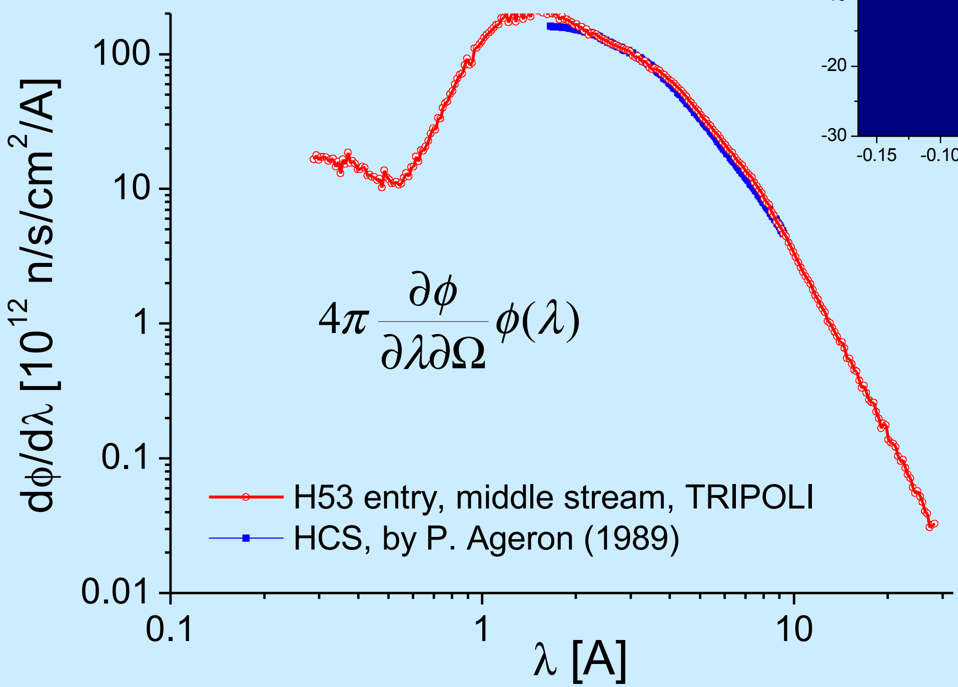
**tools for**

- simulation of absolute neutron flux
- Resolution and intensities for inelastic scattering and powder diffraction
- numerical optimization for any of ~ 280 instrument parameters

# Source definition: lookup tables

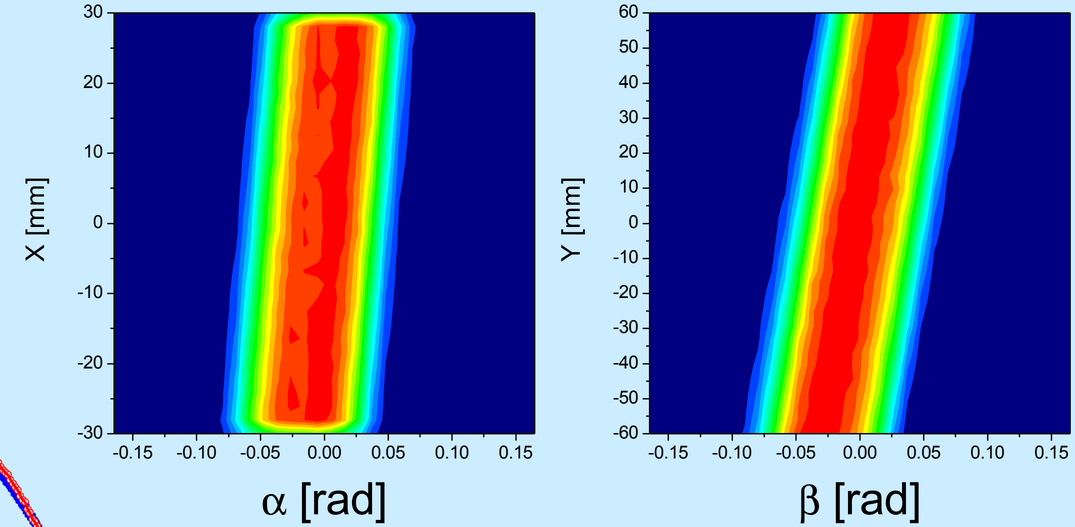
Resampling TRIPOLI data for H53:

in the middle stream




$$4\pi \frac{\partial \phi}{\partial \lambda \partial \Omega} \phi(\lambda)$$

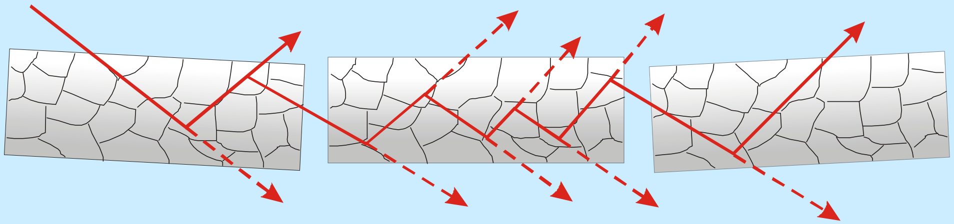
*horizontal* *vertical*




used as look-up tables
in RESTRAX ⇒

# Mosaic and gradient crystals

- **Random-walk model for secondary extinction**



Tilted segments of mosaic crystals

Migration between segments

Optional uniform lattice gradient - theoretical model by Hu H.-C., *J. Appl. Cryst.* **26**, 1993, 251-257.

Absorption - capture, TDS, incoherent scattering by Freund A. K., *Nucl. Instr. Meth.* A **213**, 1983, 495-501.

- Sampling procedure

Mosaic distribution: $g(\Delta\theta)$

- **Random walk steps: *Δt***

***mosaic***

$$\Delta t = -\log\left(1-\xi\cdot P_{seg}\right)/Q_{kin}\,g(\Delta\theta)$$

***mosaic & gradient***

$$\Delta t = \frac{\eta}{grad\theta}\,erf^{-1}\left[erf(\Delta\theta)-\frac{grad\theta}{Q_{kin}}\cdot\log\left(1-\xi\cdot P_{seg}\right)\right]$$

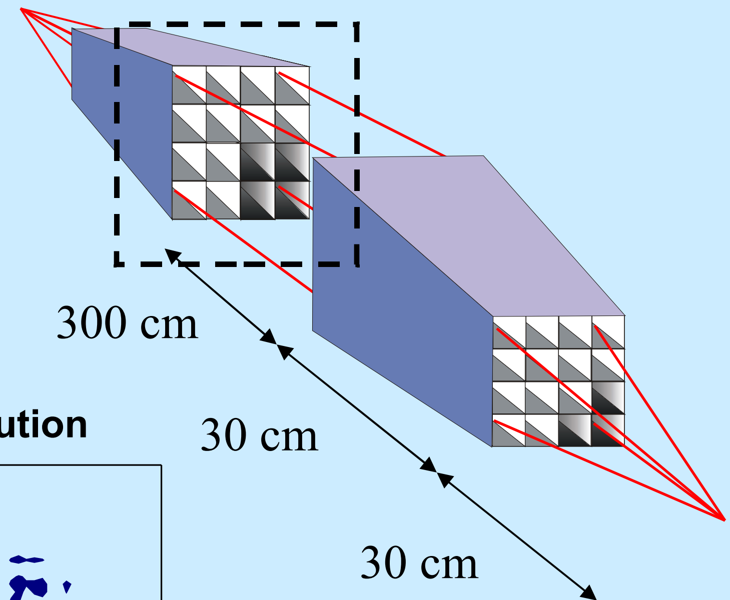
where $P_{seg}$ is the total scattering probability for 1 segment

# Multichannel parabolic & elliptic guides

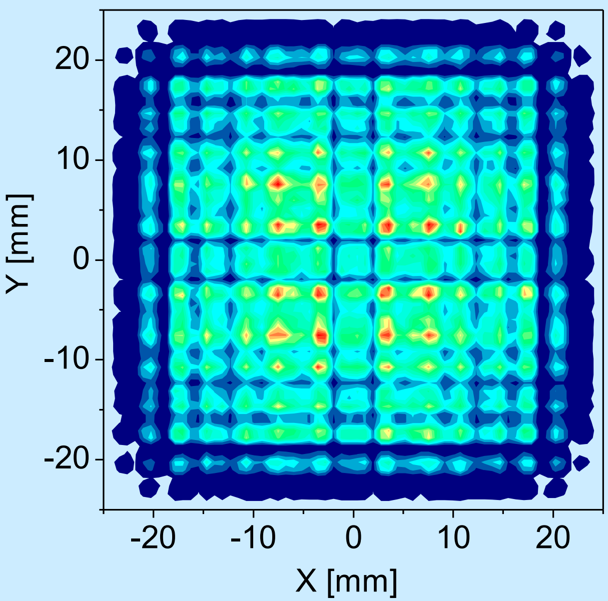
**Test:** point to point focusing:

*guides:* 21x21 slots, space 1.8 mm,
lam. thickness 0.2 mm, *m*=3

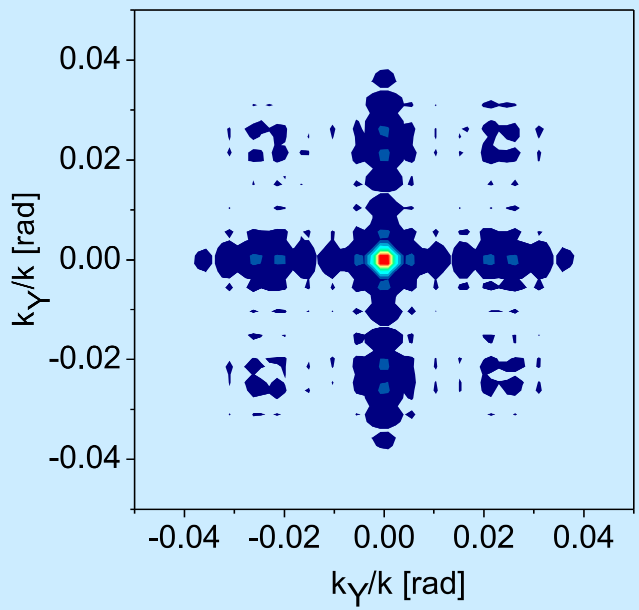
*source:* 1x1 mm$^2$, $\lambda$=4.5 A




**spatial distribution**




**angular distribution**



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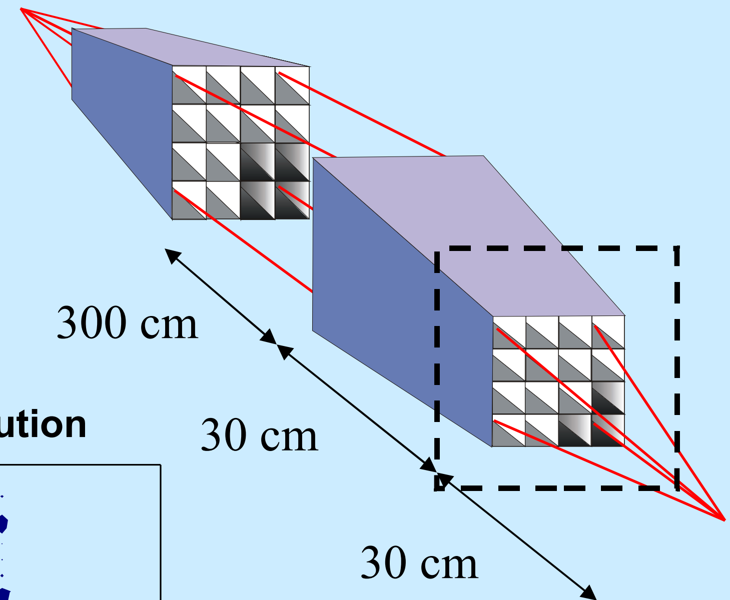
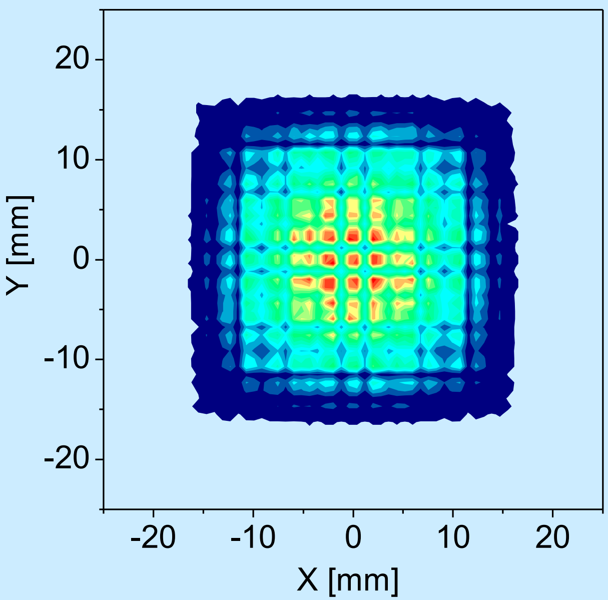
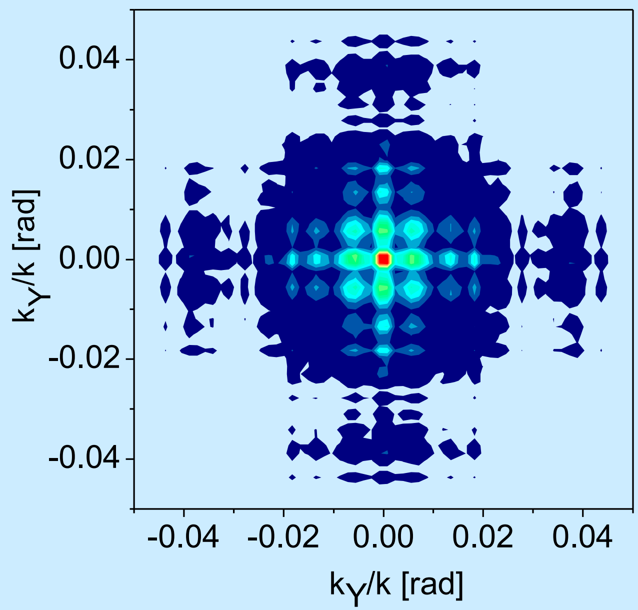



**spatial distribution**




**angular distribution**



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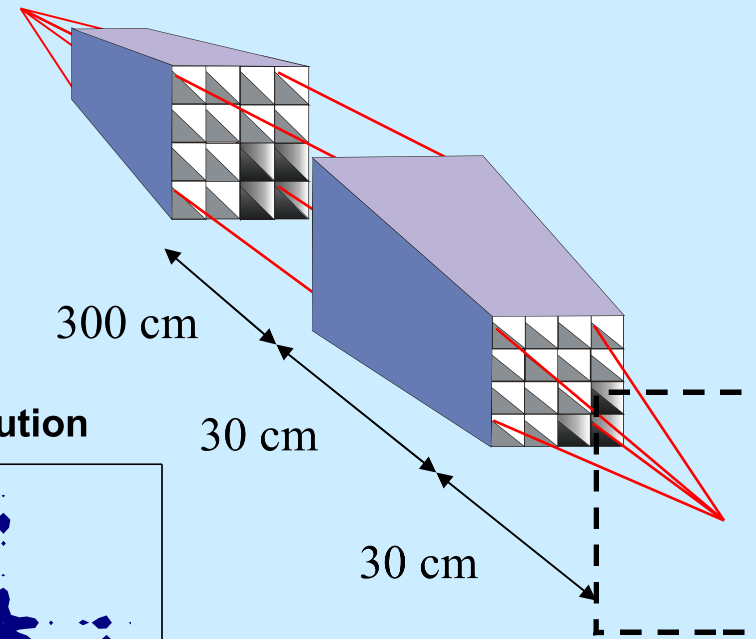
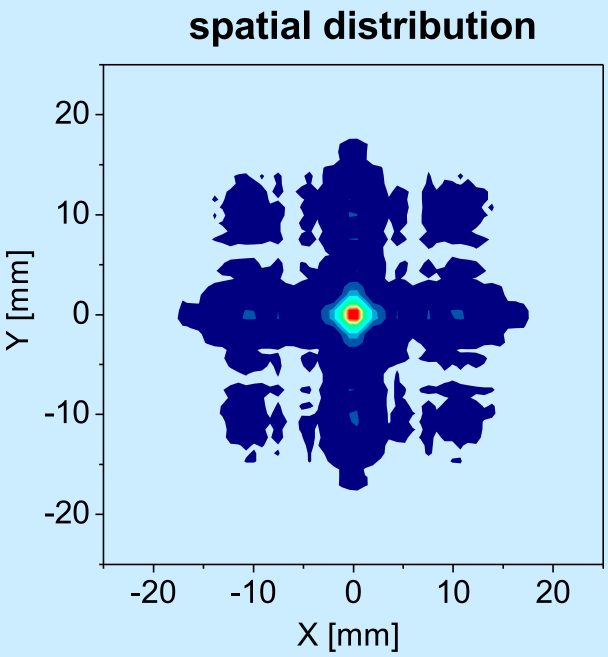
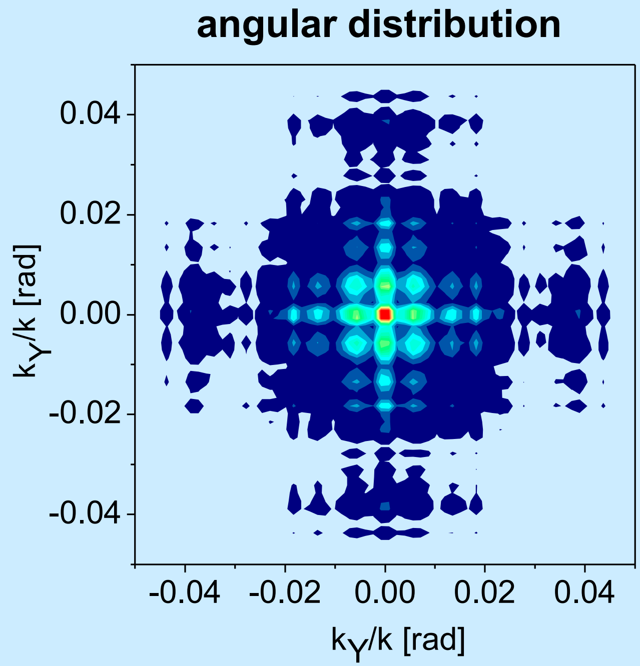
<u>*source:*</u> 1x1 mm$^2$, $\lambda$=4.5 A



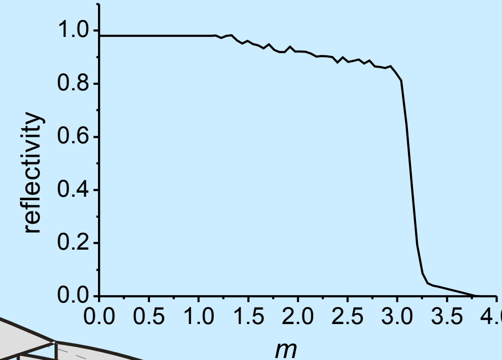
# Multichannel guide & focusing monochromator

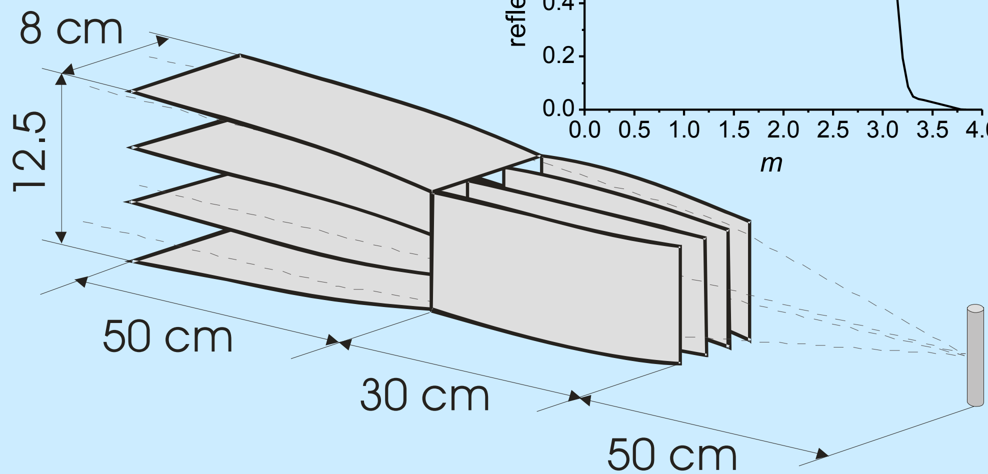
## TAS - IN14 setup

- cold source
- straight $^{58}$Ni guide, 6x12 cm$^2$
- monochromator: PG 002, doubly focusing, $\lambda$=4.05 Å
- target (sample) area: 3x3 mm$^2$
- *optimisation:* crystal curvatures

## Multichannel guide

- 20 (hor.) or 30 (ver.) blades
- thickness 0.5 mm
- *m*=3 supermirror (concave sides)
- elliptic & parabolic profiles
- *optimisation:* entry & exit width

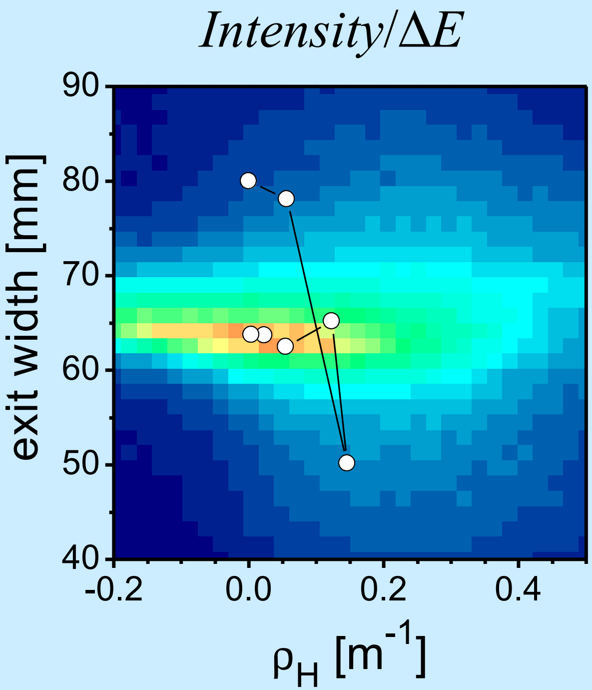


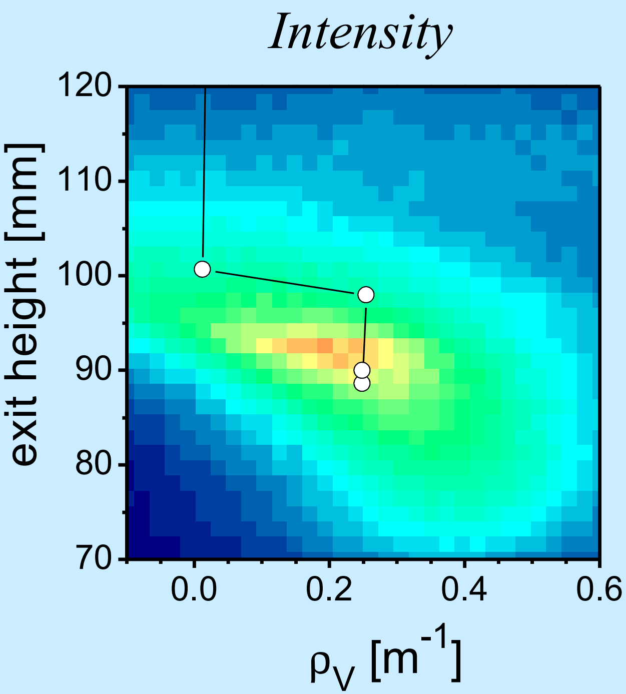
# Mapping of parameter space

Multiple instrument parameters can be optimized simultaneously

Example for parabolic guide exit width/height and monochromator curvature



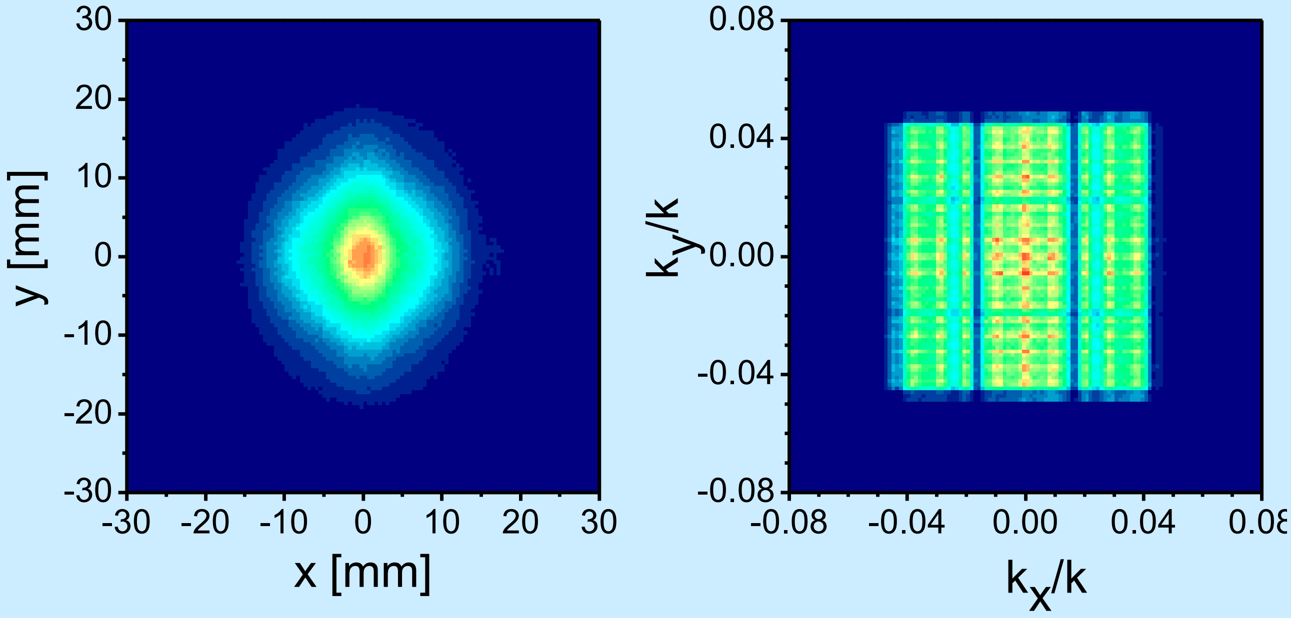

**horizontal**



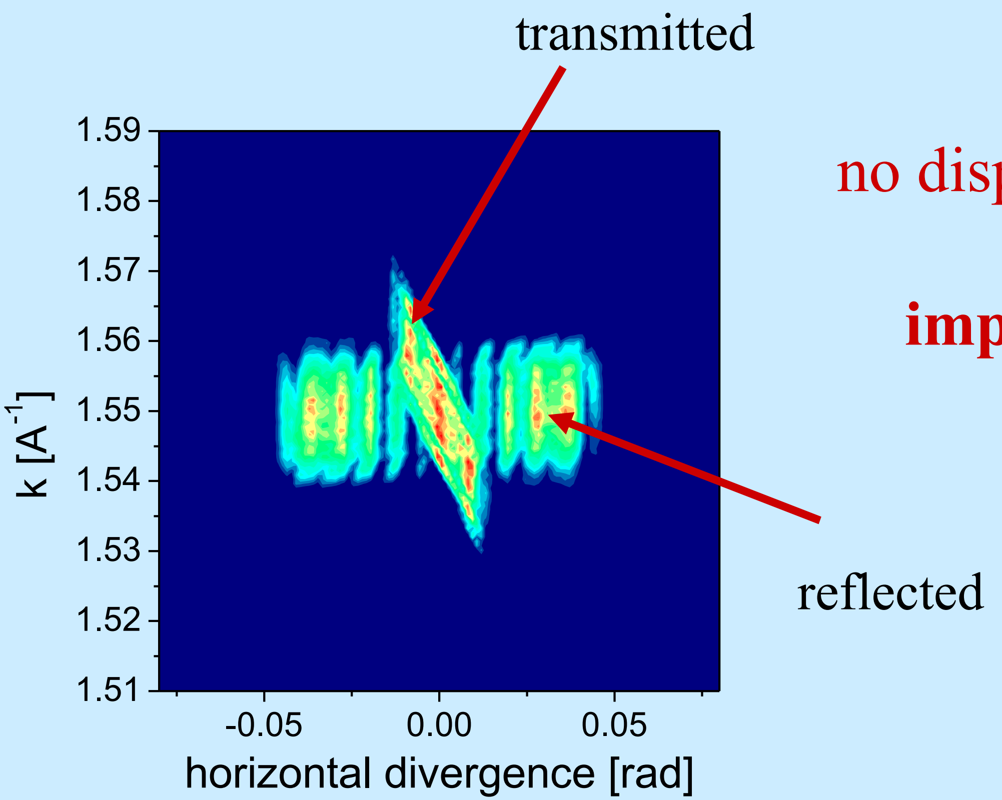

**vertical**

# Multichannel guide & focusing monochromator

## Parabolic blades



# Incident beam in *k*-space




no dispersion of reflected neutrons

=>

**improved energy resolution**

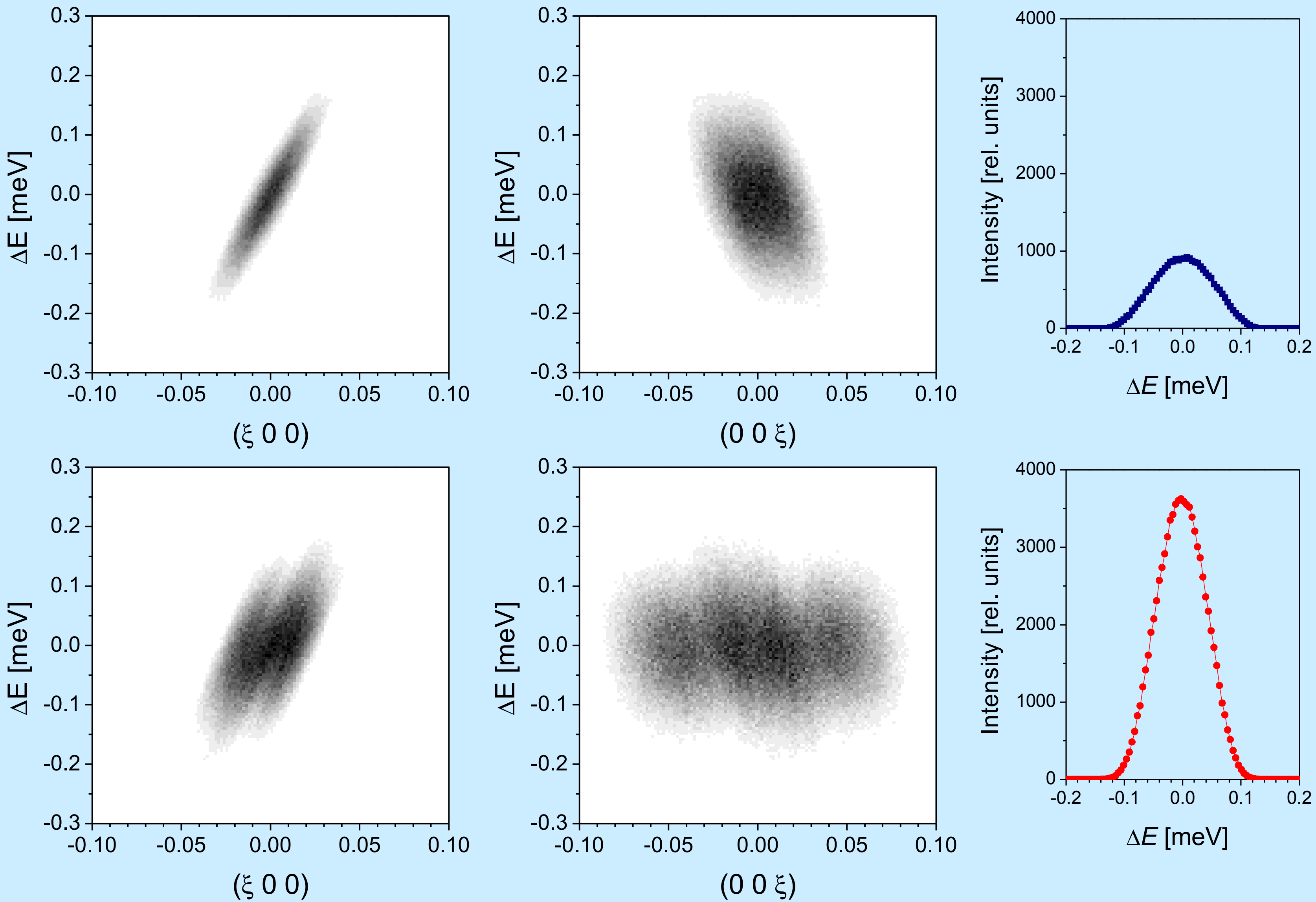
**Sample at the focal point:**

the guide selects quasi-parallel beam after the monochromator

# Resolution function

no guide

multichannel guide



# Concluding remarks

Plans for future development

- GUI for SIMRES
- merging the ray-tracing codes of RESTRAX and SIMRES in a single kernel
- splitting code into client and server parts
- further development of neutron optics elements