AB-INITIO MONTE CARLO SIMULATIONS OF RELATIVISTIC PARTICLE SCATTERING AND RADIATION IN ORIENTED CRYSTALS

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Outline

- **CRYSTAL** simulation code for particle tracking in crystal.
  - **General description** and main options
  - Model of **Coulomb scattering** on atoms
  - High performance computing using **OpenMPI**
- Simulation of charged beam deflection by a bent crystal
  - **855 MeV electron** beam deflection in silicon and germanium crystals (111)* at **Mainz Microtron MAMI**
  - **e^+/e^- 120 GeV** beam deflection in silicon and germanium crystals at **CERN SPS H4**: stochastic deflection
  - Simulation of recenty observed **quasichanneling oscillations** in the deflection angle distribution at **SLAC**
  - Simulation of **multilple volume reflection** at the **FCC** energy
- Simulation of the crystal-based collimation experiment at the LHC

CRYSTAL simulation code*

Main conception – tracking of charged particles in a crystal in averaged atomic potential

Program modes:

- **1D** model – particle motion in an interplanar potential
- **2D** model – particle motion in an interaxial potential

Simulation of the different physical processes:

- Multiple and single Coulomb scattering on nuclei and electrons.
- Nuclear scattering (elastic, quasielastic, inelastic)
- Ionization energy losses
- Crystal geometry (entrance/exit through the crystal lateral surface; miscut angle)

Radiation by Baier-Katkov formula (L. Bandiera's talk)

Accelerator routine for crystal-based collimation with implementation of:

- Both betatron and synchrotron oscillations
- Map of absorbers with transverse aperture, Twiss parameters and dispersion functions

Advantages:

- Spline interpolation of main functions => high calculation speed (up to 10^3 particles/s/core)
- Setting all the properties of crystal material and lattice in input files => algorithm universality
- Varying initial parameters of both crystal and incoming beam => optimization problem
- OpenMPI parallelization for high performance compiting

*A.I. Sytov, Vestnik. Belarusian. Univ. Series 1 N2 (2014), 48-52, (in Russian).
A.I. Sytov, V.V. Tikhomirov. NIM B 355 (2015) 383–386.

CRYSTAL simulation code: the model of Coulomb scattering on atoms*

We use **Yukawa potential** for the cross-section of scattering on atoms:

$$\frac{d\sigma}{d\Omega} = \frac{Z^2\alpha^2}{p^2\beta^2}\frac{1}{(\vartheta^2+\vartheta_1^2)^2}\,, \qquad (1)$$

where

$$\vartheta_1 = \frac{\hbar}{p\,a_{TF}}\left[1.13 + 3.76(\alpha Z/\beta)^2\right]^{1/2} \qquad (2)$$

We divide the **Coulomb scattering** process onto **multiple** and **single scattering**:

- **Multiple scattering $\vartheta \leq \vartheta_2$**:

$$\left\langle \vartheta_s^2(z) \right\rangle / dz = n_N \int_0^{\vartheta_2} \int_0^{2\pi} \frac{d\sigma}{d\Omega}[1 - \exp(-p^2\vartheta^2 u_1^2)]\, d\varphi \vartheta d\vartheta\,, \qquad (3)$$

where the exponent represents the **Debye-Waller factor**, describing incoherent scattering suppression first predicted by **M.L. Ter-Mikaelian****

- **Single scattering $\vartheta > \vartheta_2$**: we calculate the angle according to (1), discarding the events in which specially generated random numbers **do not exceed** the value of the **Debye-Waller factor**.

*V.V. Tikhomirov. arXiv 1502.06588v1

** M. L. Ter-Mikaelian, High-energy electromagnetic processes in condensed media. Wiley. New York, 1972.

High performance computing with CINECA supercomputers by CRYSTAL using OpenMPI

MPI communications in CRYSTAL

- **MPI Broadcast:** to send the input data to all the processes, read by the first one
- **MPI Reduce:** to collect the integral values (channeling efficiency, inelastic loss rate, number of passage through the crystal, etc.) and to find the total or average value (can be turned off)

	CPU	Totalcores/ Total Nodes	Peak perfor-mance,PFlop/s	Memory per node	Accelerators
FERMI	PowerA2@1.6GHz, 16 cores each	163840/ 10240	2	16 GB	-
MARCONI-A1	Intel Broadwell 2x Intel Xeon E5-2697 v4@2.3 GHz 18 cores each	54432 / 1512	2	128 GB	-
GALILEO	Intel Haswell 2 x Intel Xeon 2630 v3@ 2.4GHz8 cores each	8384 / 524	1	128 GB	Intel Phi 7120p/ NVIDIA K80

Max number of cores used simultaneously by CRYSTAL

- **FERMI**: **2048**
- **GALILEO**: **768**
- **MARCONI-A1**: **2152**

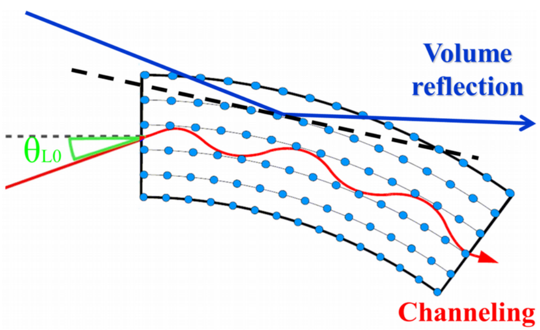
What have we been granted by?

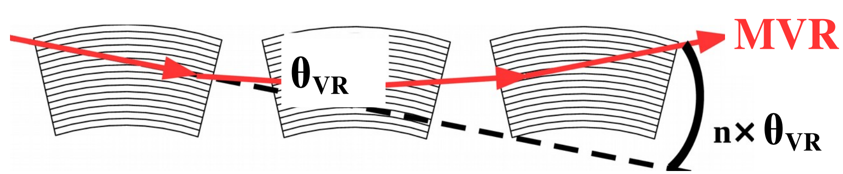
- **FERMI**: **200 kh**
- **GALILEO**: **100 kh**
- **MARCONI-A1**: **29 kh**

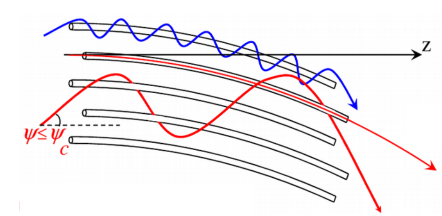
Principle investigator: E. Bagli

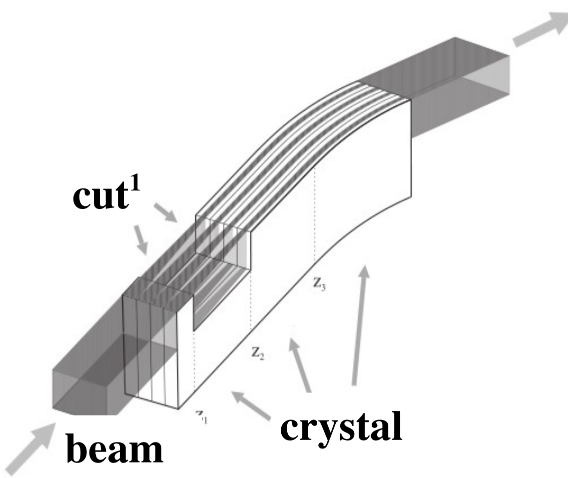
Coherent effects of particle deflection in a bent crystal simulated by CRYSTAL

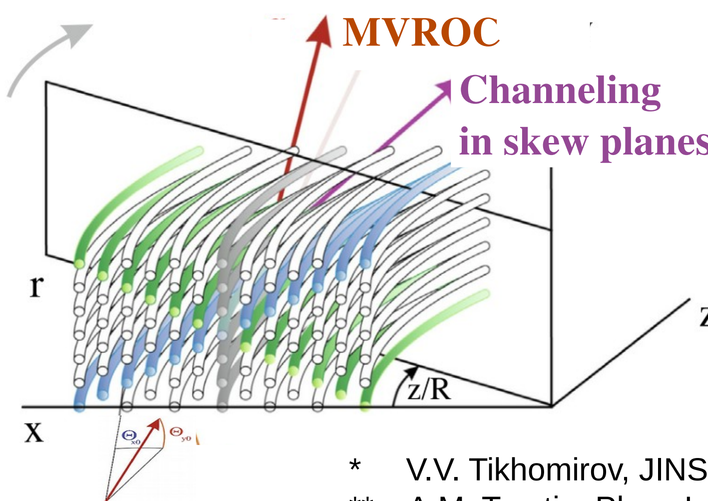
- **Planar effects:** channeling, channeling in a crystal with a narrow plane cut*, volume reflection**, multiple volume reflection in a crystal sequence (MVR)
- **Axial effects:** axial channeling, stohastic deflection***, planar channeling in skew crystal planes, multiple volume reflection in one bent crystal (MVROC)****



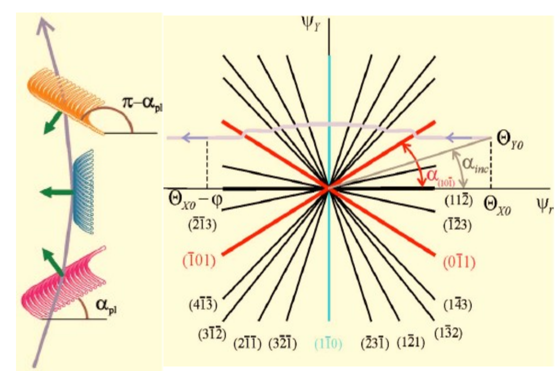








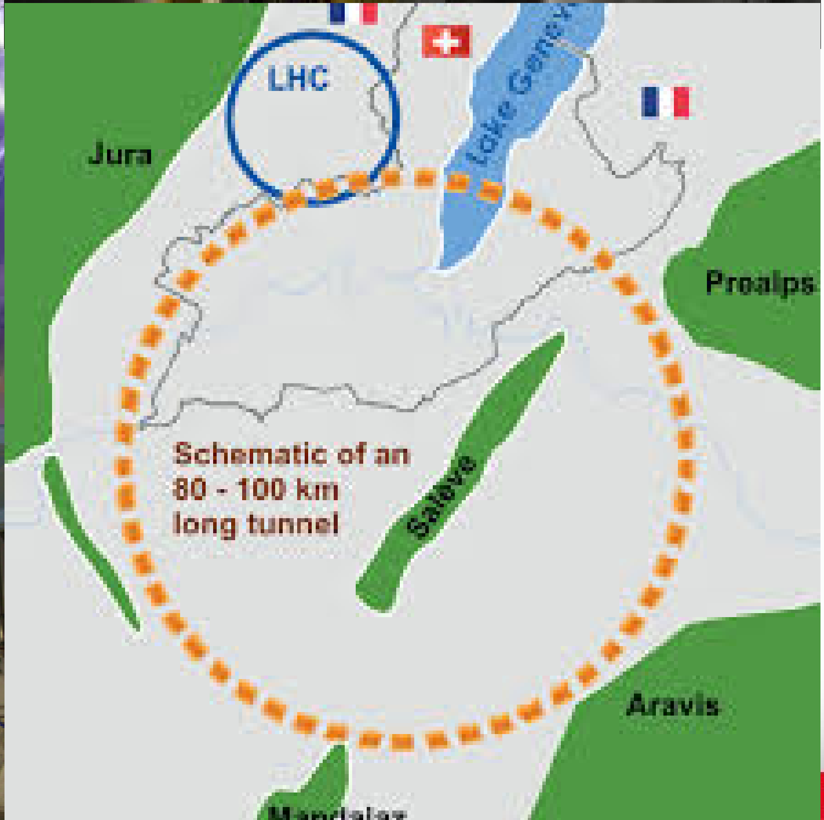
MVROC: reflection from different planes



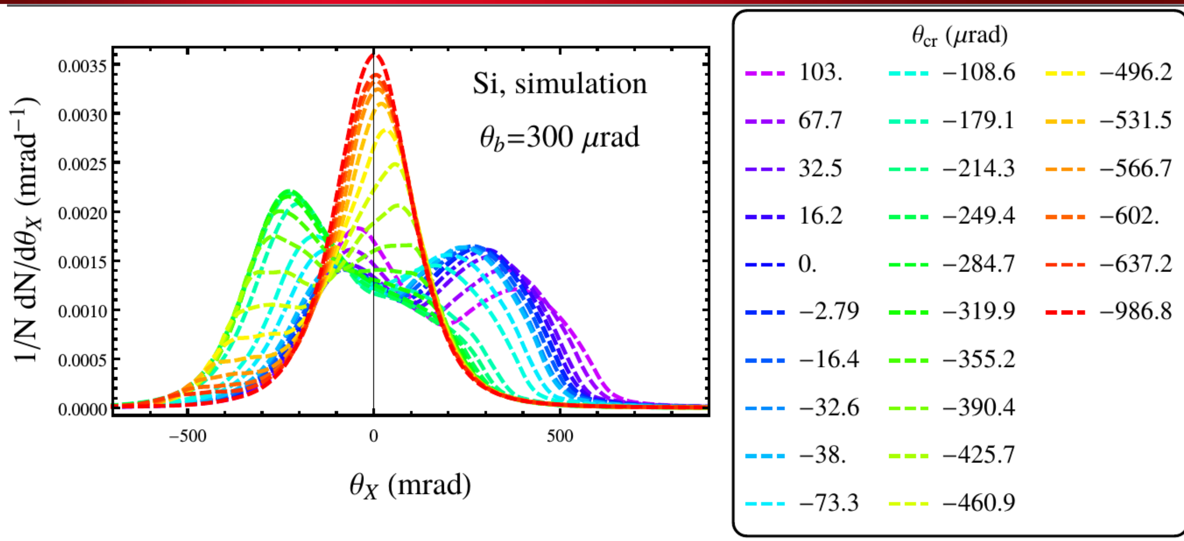
* V.V. Tikhomirov, JINST 2 (2007) P08006.
** A.M. Taratin, Phys. Lett. A 119 N8 (1987) 425-428.
*** N.F. Shul'ga, A.A. Greenenko, Phys. Lett. B 353 (1995) 373–377.
**** V.V. Tikhomirov, Phys. Lett. B V. 655 (2007) 217-222.

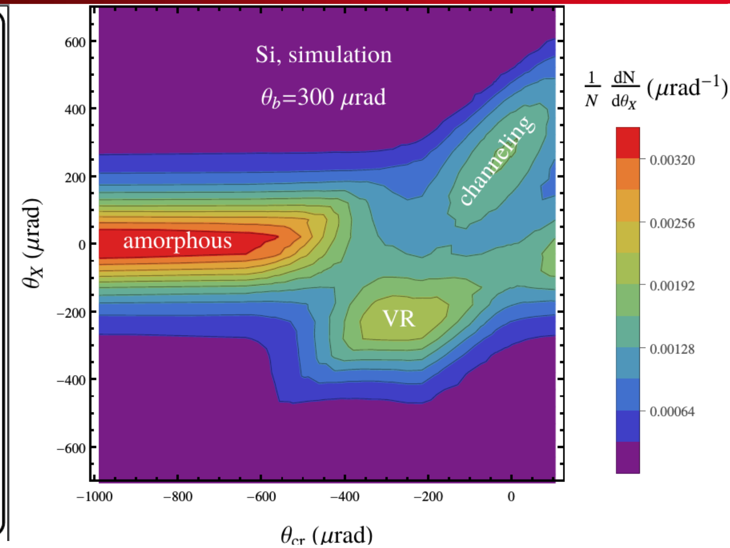
Simulation of beam deflection experiments

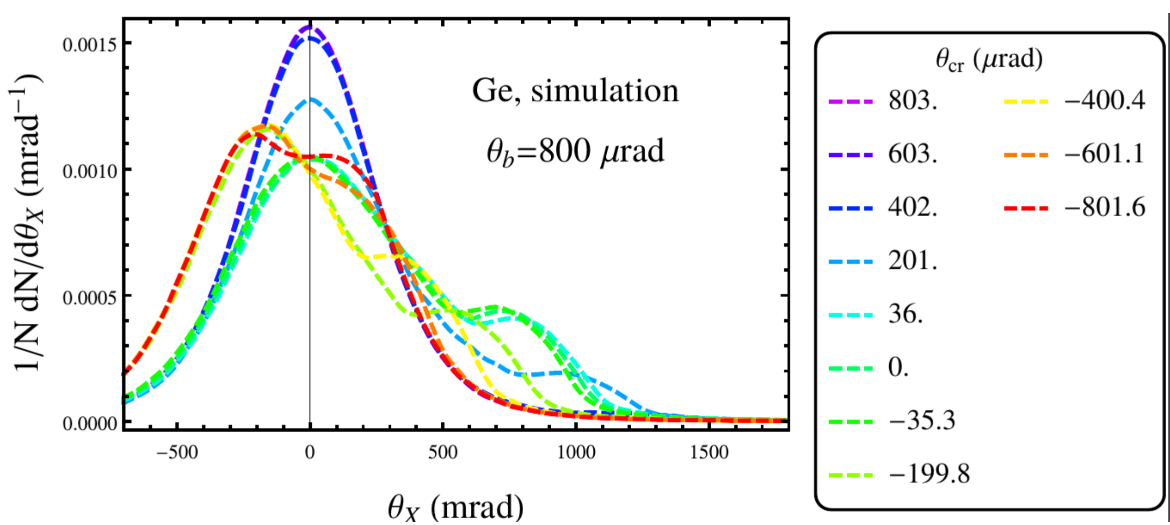


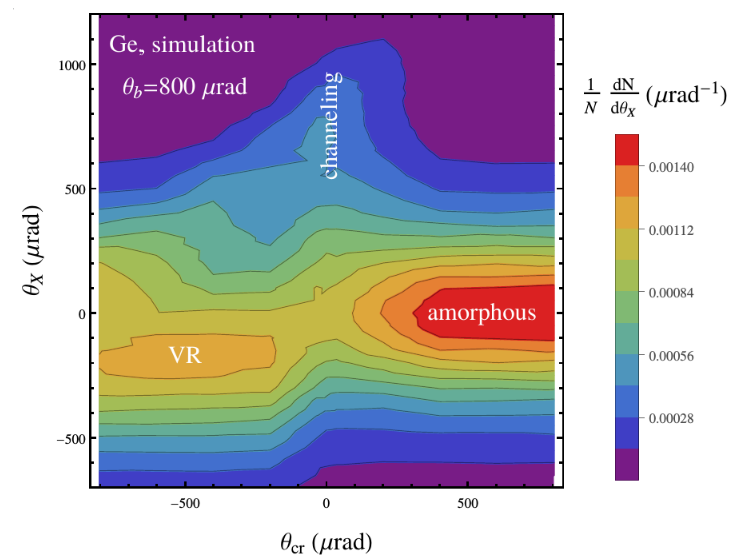



Simulations of beam deflection in silicon and germanium crystals (111)* at Mainz Microtron MAMI: angular scan



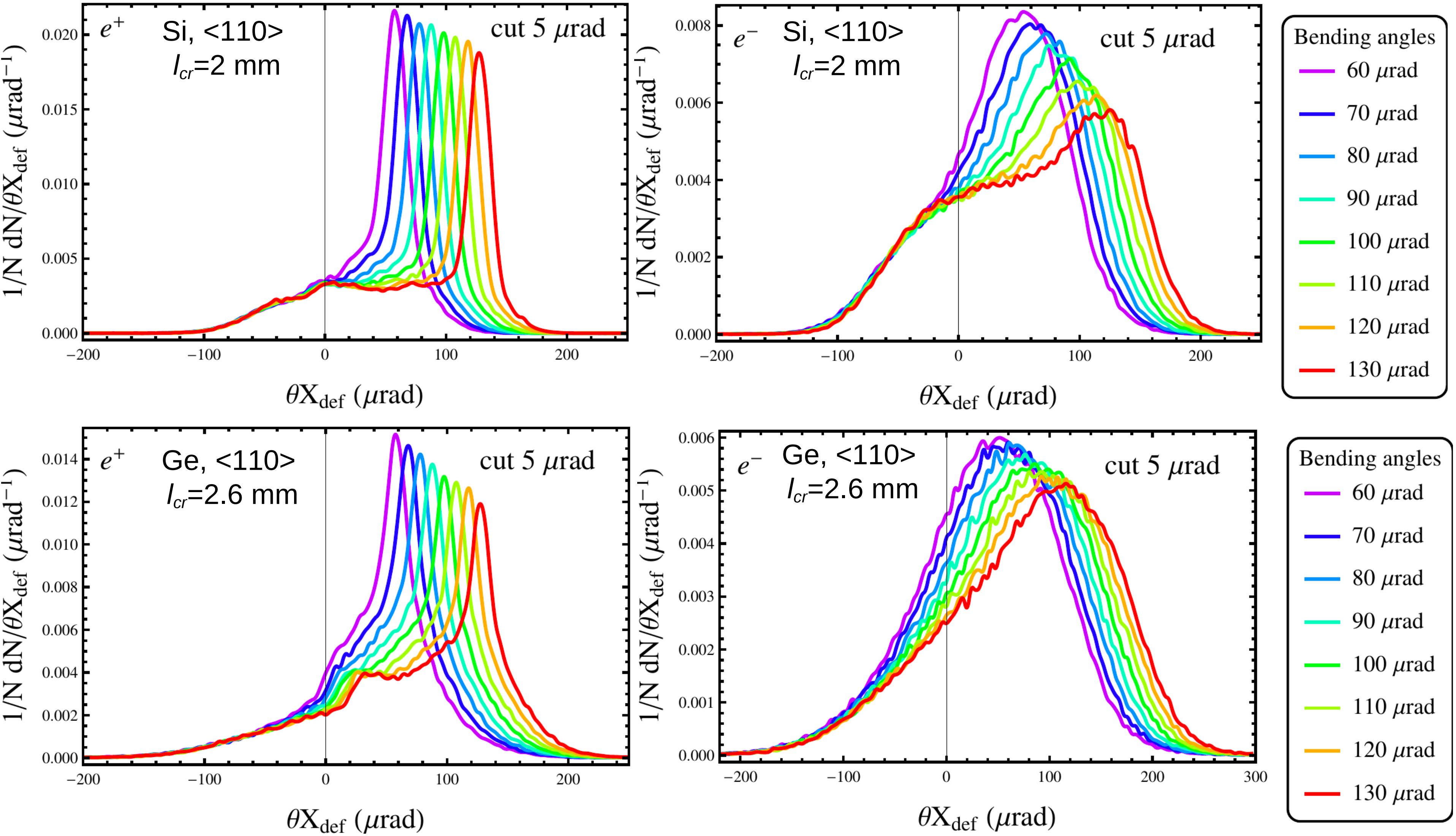






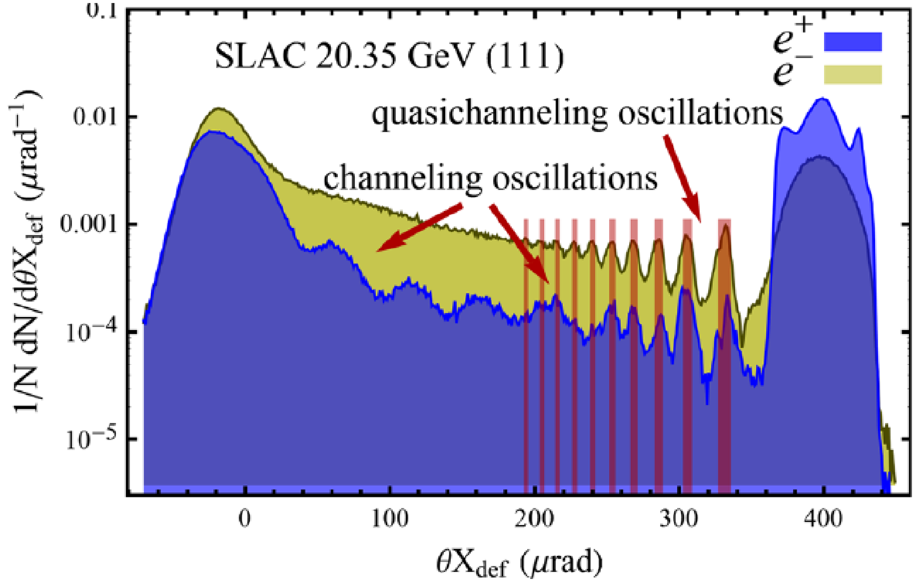
*D. De Salvador et al. "Steering efficiency and dechanneling of a Sub-GeV electron beam as a function of curvature and energy", this conference

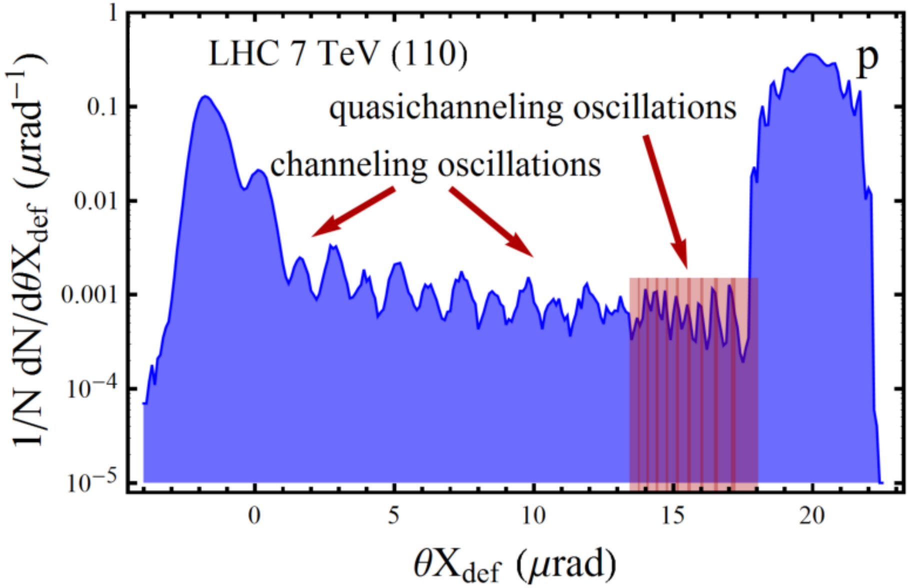
Simulations of e^+/e^- 120 GeV beam deflection in silicon and germanium crystals at CERN SPS H4: stochastic deflection*

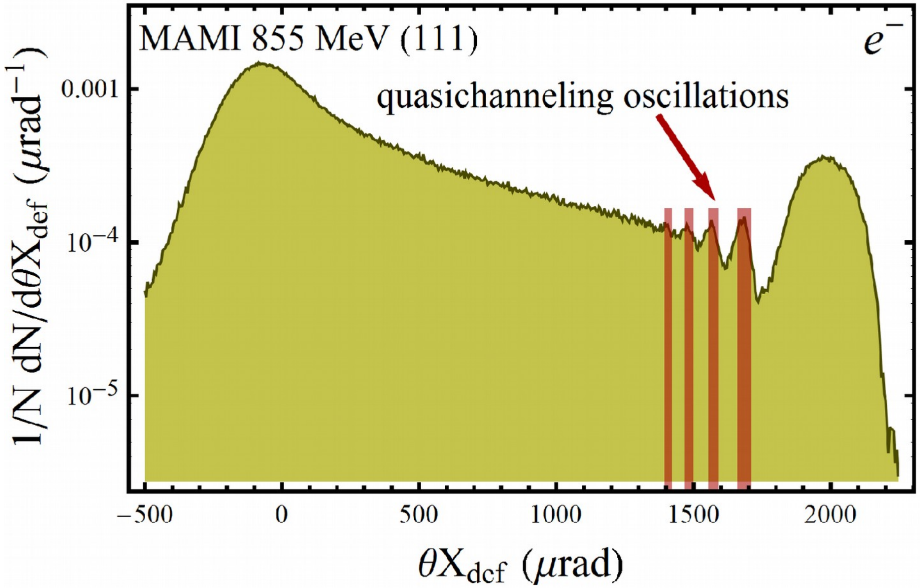


*N.F. Shul'ga, A.A. Greenenko, Phys. Lett. B 353 (1995) 373–377.
L. Bandiera et al. Eur. Phys. J. C (2016) 76:80.

Planar channeling and quasichanneling oscillations In the deflection angle distribution*







Interpeak distance

- **Channeling oscilations:**

$$\Delta\varphi_{peak} = \frac{\lambda}{2R} = \frac{\pi d_0}{2R}\sqrt{\frac{pv}{2U_0}}$$

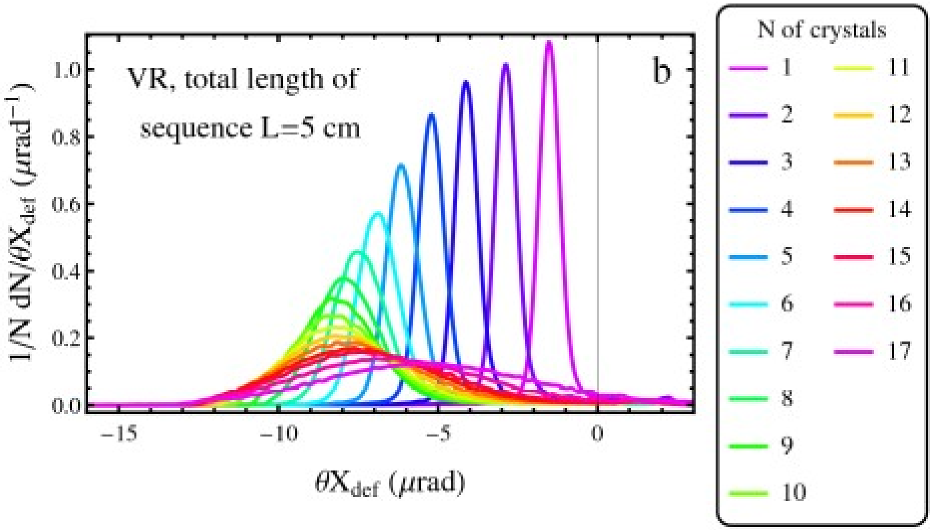
- **Quasichanneling oscilations:**

$$\Delta\varphi_{peak} = \sqrt{\frac{2d_0}{R} + (\theta_b - \theta_{Xdefl})^2} - (\theta_b - \theta_{Xdefl}) \approx \frac{d_0}{R(\theta_b - \theta_{Xdefl})}$$

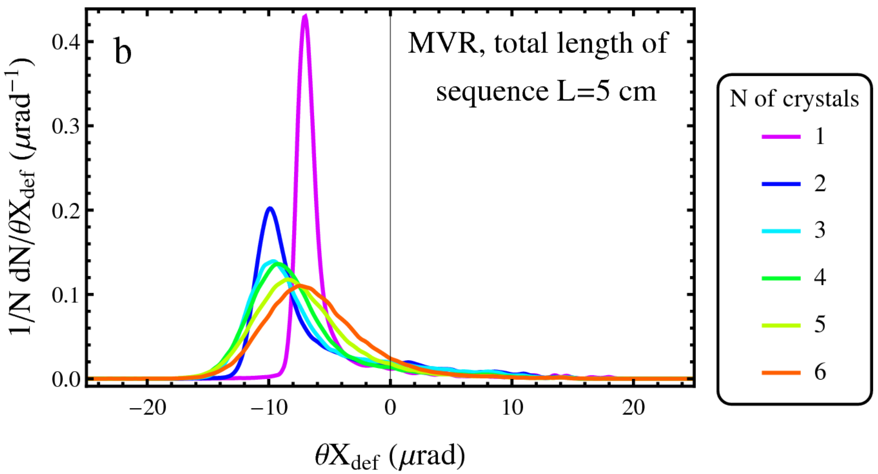
*A.I. Sytov, V. Guidi, V.V. Tikhomirov et al. Eur. Phys. J. C 76:77 (2016).
A.I. Sytov, V.V. Tikhomirov. NIM B 355 (2015) 383–386.
Poster session PS3-18
U. Wienands' talk

Simulation of beam deflection by a bent crystal for a possible crystal-based collimation system at the Future Circular Collider

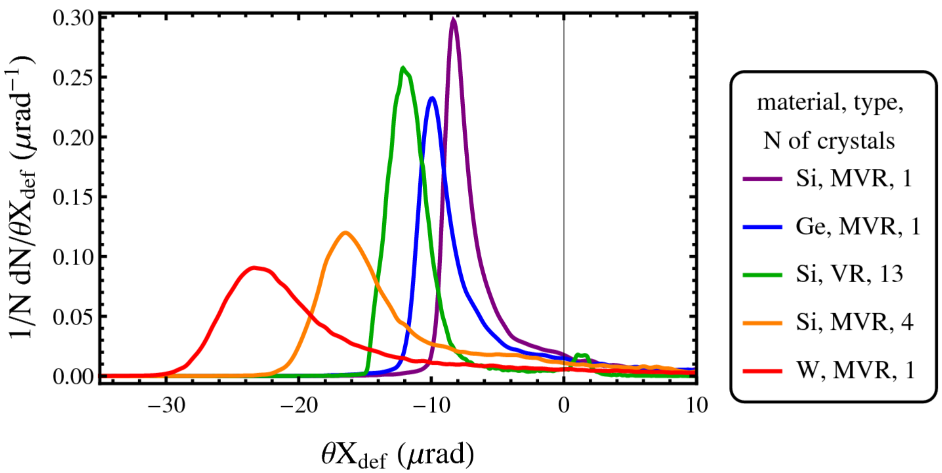
Multiple volume reflection in a crystal sequence



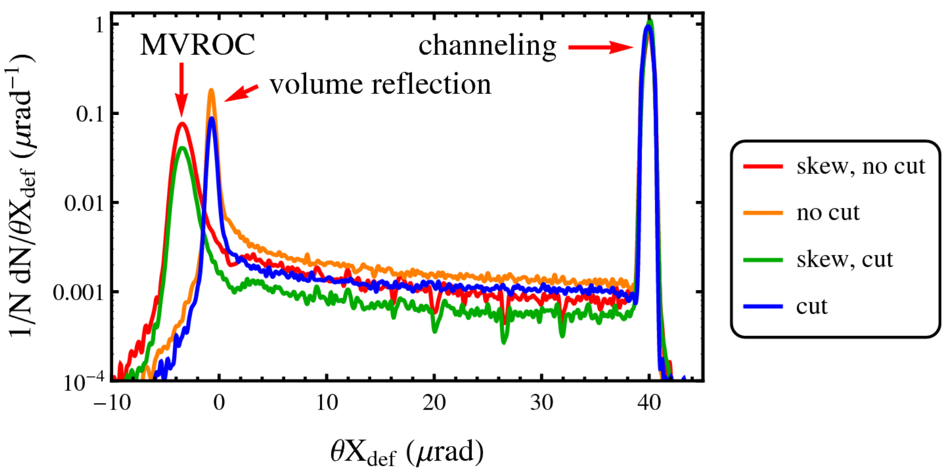
MVROC in a crystal sequence



MVROC in Si, Ge and W

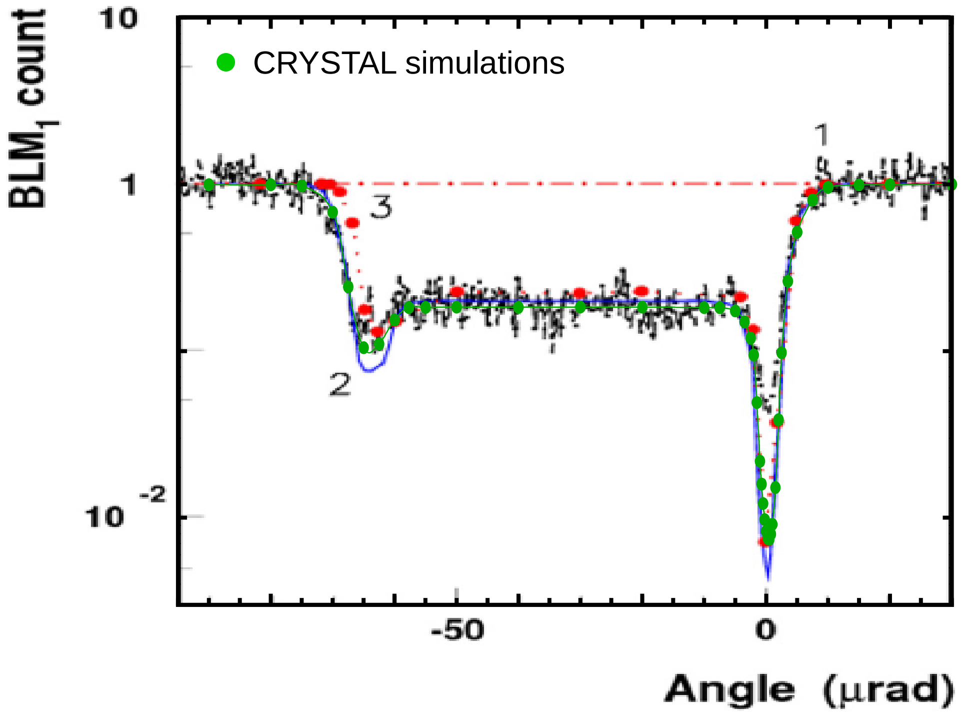


Channeling in skew crystal planes and in a crystal with a cut



Simulation of the crystal-based collimation experiment at the LHC

Inelastic losses *vs* crystal orientation

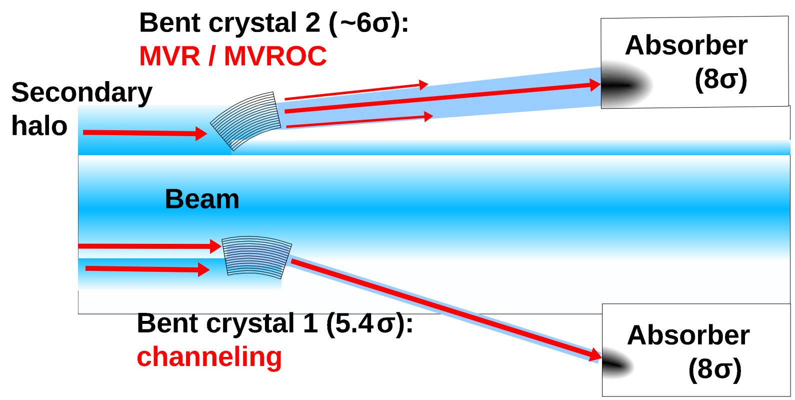


LHC run II setup references

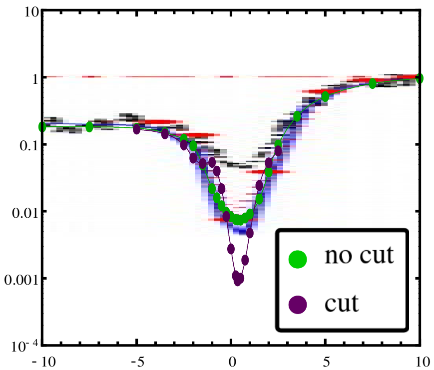
- W. Scandale et al. Phys. Lett. B 758 (2016) 129-133
- D. Mirarchi, Crystal collimation for LHC, PhD thesis, CERN-THESIS-2015-099, 2015.
- LHC Optics Web Home, http://lhc-optics.web.cern.ch/lhc-optics/www/
- R. Bruce arXiv: 1410.5990v1 [physics.acc-ph] 22 Oct 2014
- K.A. Olive et al. (Particle Data Group), Chin. Phys. C, 38, 090001 (2014) and 2015 update.

Ways to improve the crystal-based collimation system:

- **Double** crystal-based collimation system (**poster session PS3-19**)



- A bent **crystal** with a **cut***



one order of inelastic losses decrease!

*V.V. Tikhomirov, JINST 2 (2007) P08006.

Conclusions

- **CRYSTAL** simulation code has been developed. It represents itself a tool for simulation of a wide number of coherent effects of charged particles deflection in a crystal, accompanied by radiation.
- A wide number of experiments at different machines (**MAMI microtron**, **CERN SPS H4**) has been simulated.
- Recently observed **quasichanneling ocsillations** have been predicted in CRYSTAL simulations.
- The different effects (**channeling** in a crystal with **cut** and **in skew crystal plane**s, **MVR in a crystal sequence**, **MVROC** and **MVROC in a crystal sequence**) for a possible crystal-based collimation system at the Future Circular Collider.
- The **LHC crystal-based collimation experiment** has been simulated.

Acknowledgements:

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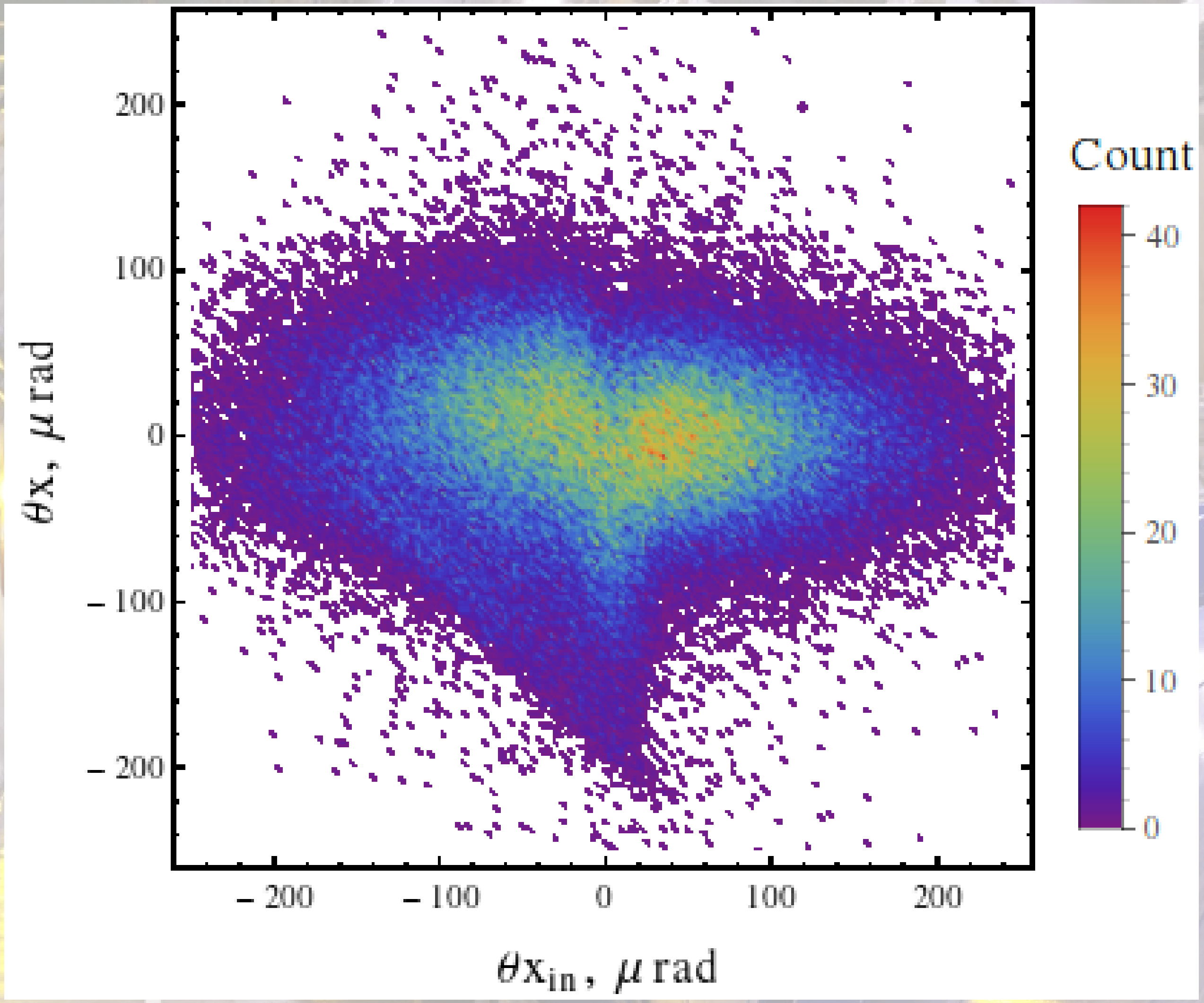

Thank you for attention!

Recent development and verification of ***simulation methods***

V. Guidi, L. Bandiera, V.V. Tikhomirov, Phys. Rev. A. 86 (2012) 042903

L. Bandiera ... V. Guidi,.. V.V. Tikhomirov , Phys. Rev. Lett. 111 (2013) 255502 .

A. Mazzolari ... V. Guidi, ..V.V. Tikhomirov , Phys. Rev. Lett. 112 (2014) 135503.

L. Bandiera ... V. Guidi,.. V.V. Tikhomirov , Phys. Rev. Lett. 115 (2015) 025504.