Istituto Nazionale di Fisica Nucleare

European Commission

www.kisti.re.kr

Korea Institute of Science and Technology Information

Trillion

Implementazione di modelli per cristalli

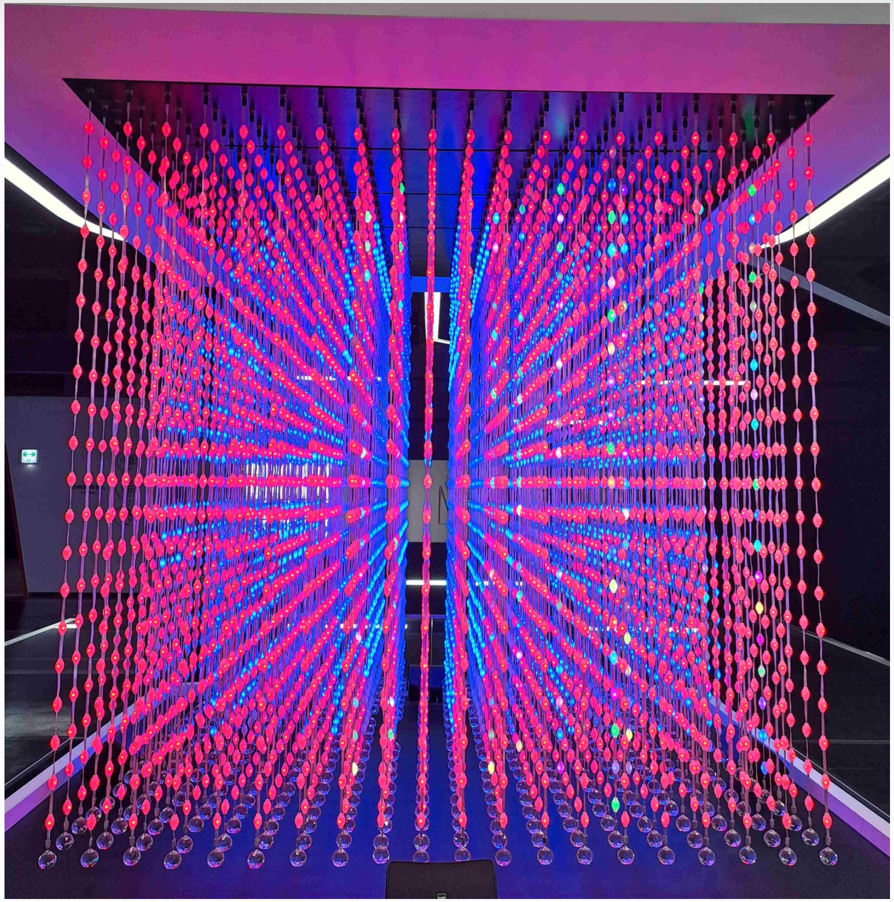
Marie Curie Global Fellowships, Project TRILLION GA n. 101032975

Dr. Alexei Sytov

In close collaboration with Dr. Gianfranco Paternò

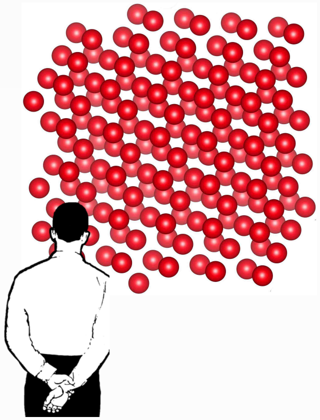
Riunione annuale Geant4INFN 05/06/2024

How an oriented crystal looks like

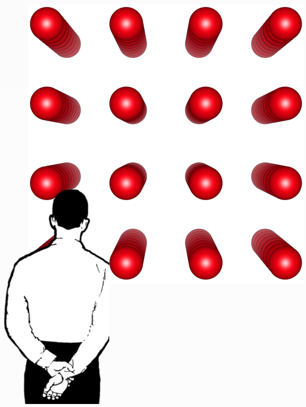


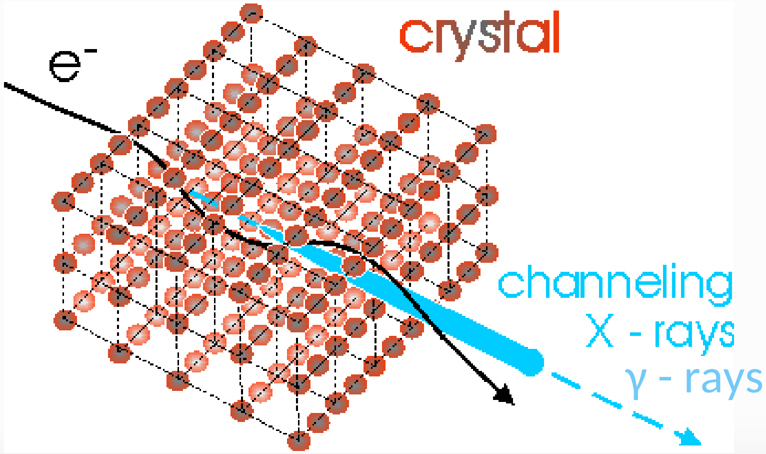
from National Science Museum, Daejeon, Korea

Non-oriented crystal



Oriented crystal





Marie Sklodowska-Curie Action Global Individual Fellowships by A. Sytov in 2021-2025, Project TRILLION GA n. 101032975

Main goal: The **implementation** of both physics of **electromagnetic processes in oriented crystals** and the design of specific applications of crystalline effects into **Geant4** simulation toolkit as Extended Examples to bring them to a large scientific and industrial community and under a free Geant4 license.

Group:

- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

Trillion

GEANT4
A SIMULATION TOOLKIT

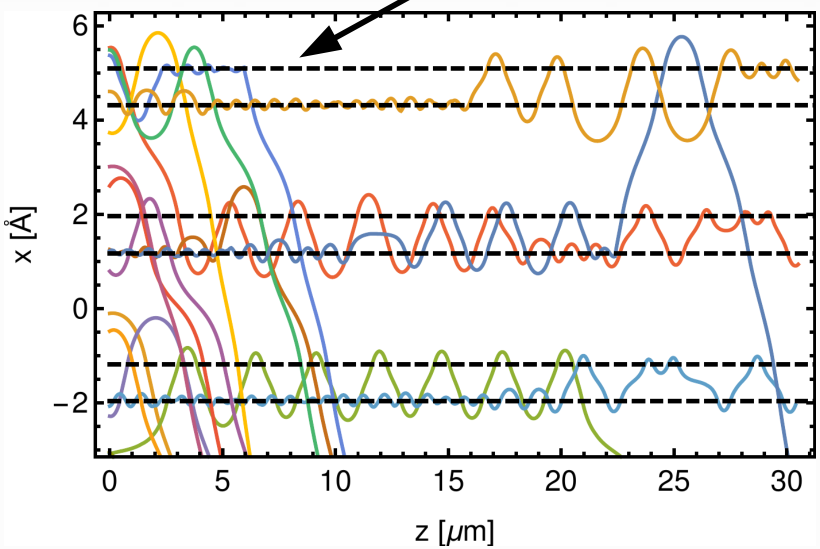
Location:

- 2 years at **KISTI** (partner organization)
- 1 year at **INFN Section of Ferrara** (host organization)
- 1 month of secondment at **IJCLab Orsay** (partner organization)
- 1 month of secondment at **DESY** (partner organization)

Baseline channeling simulation technique: CRYSTALRAD Monte Carlo simulation code

Main conception – simulation of classical trajectories of charged particles in a crystal in averaged atomic potential of planes or axes. Multiple and single **scattering simulation** at every step

Crystal planes

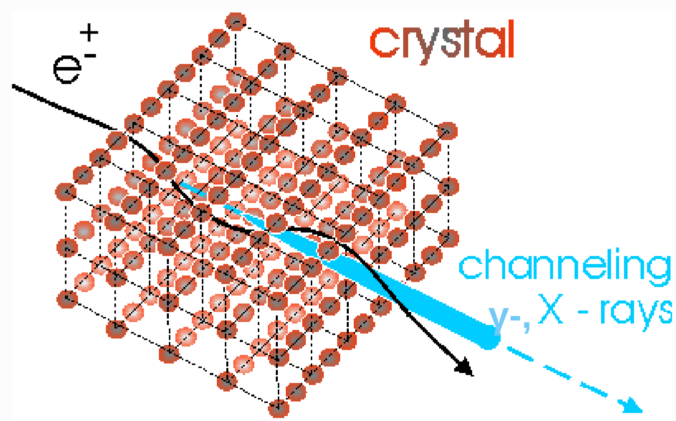


channeling*

Advantages:

- High calculation speed
- **MPI** parallelization for high performance computing

New 2024: ionization losses in channeling



Baier-Katkov formula:
integration is made over the classical trajectory

$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{[(E^2+E'^2)(v_1 v_2 - 1) + \omega^2/\gamma^2]}{2E'^2} e^{-ik'(x_1-x_2)}$$

A.I. Sytov, V.V. Tikhomirov. NIM B 355 (2015) 383–386.
L. Bandiera, et al., Nucl. Instrum. Methods Phys. Res., Sect. B 355, 44 (2015)
***A. Sytov et al. Journal of the Korean Physical Society 83, 132–139 (2023)**
A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

Current status

In Geant4 since geant4-11.2.0 !

geant4-v11.2.0/source/parameterisations/channeling/

Please use it!

https://geant4.web.cern.ch/download

Don't hesitate to contact me in the case of any problems/issues/suggestions

sytov@fe.infn.it

Geant4 Physics Reference Manual:

https://geant4-userdoc.web.cern.ch/UsersGuides/PhysicsReferenceManual/html/solidstate/channeling/channeling_fastsim.html

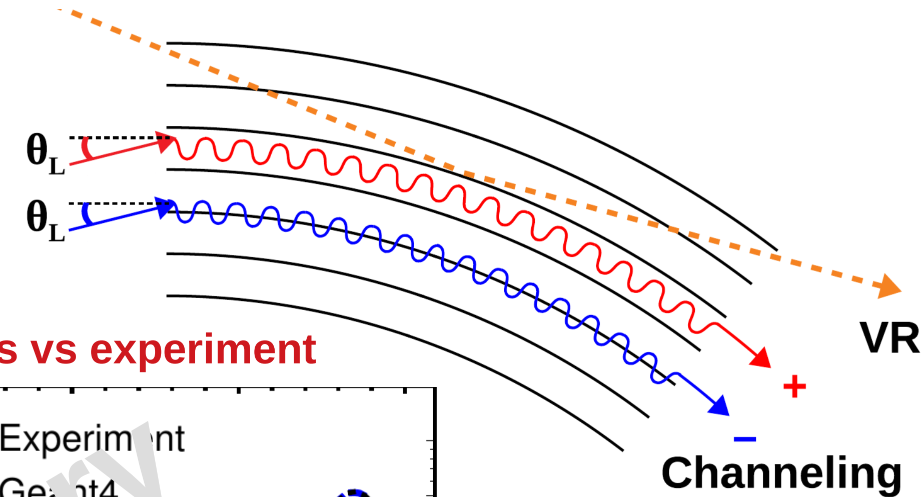
Please cite our papers if you use our model:

1. A. Sytov et al. Journal of the Korean Physical Society 83, 132–139 (2023)
2. A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

More Geant4 channeling model validation: quasichanneling oscillations* at SLAC FACET Facility

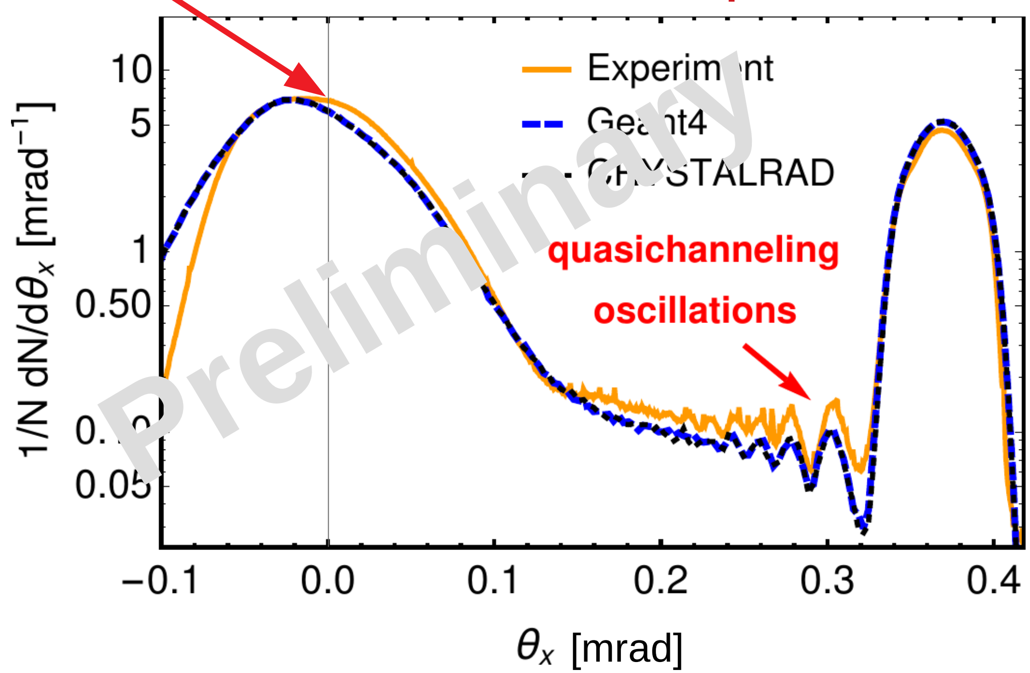
20.35 GeV positrons

60 µm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



channeling

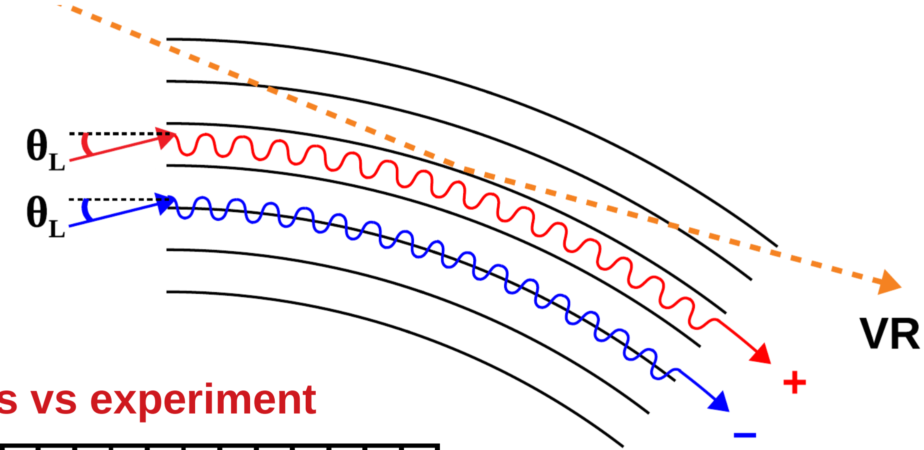
To be submitted for publication soon

*T. N. Wistisen, ..., and A. Sytov, Phys. Rev. Lett. 119, 024801 (2017)

Geant4 channeling model validation: beam deflection by a bent crystal

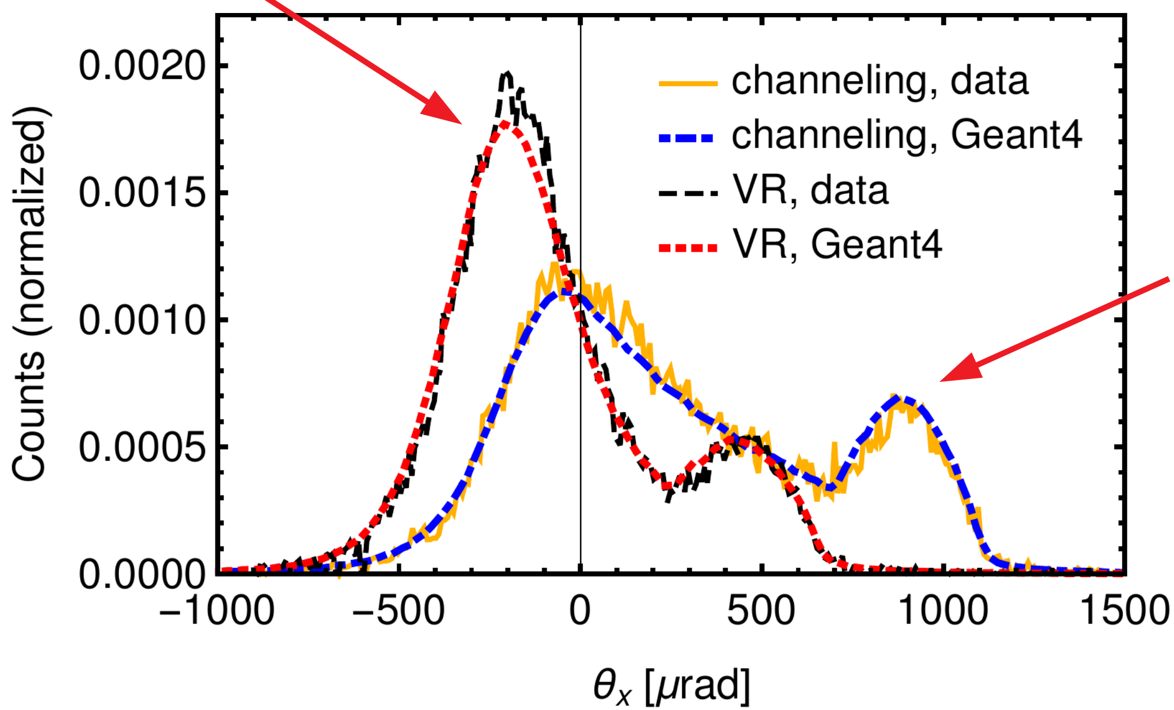
855 MeV electrons

15 µm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



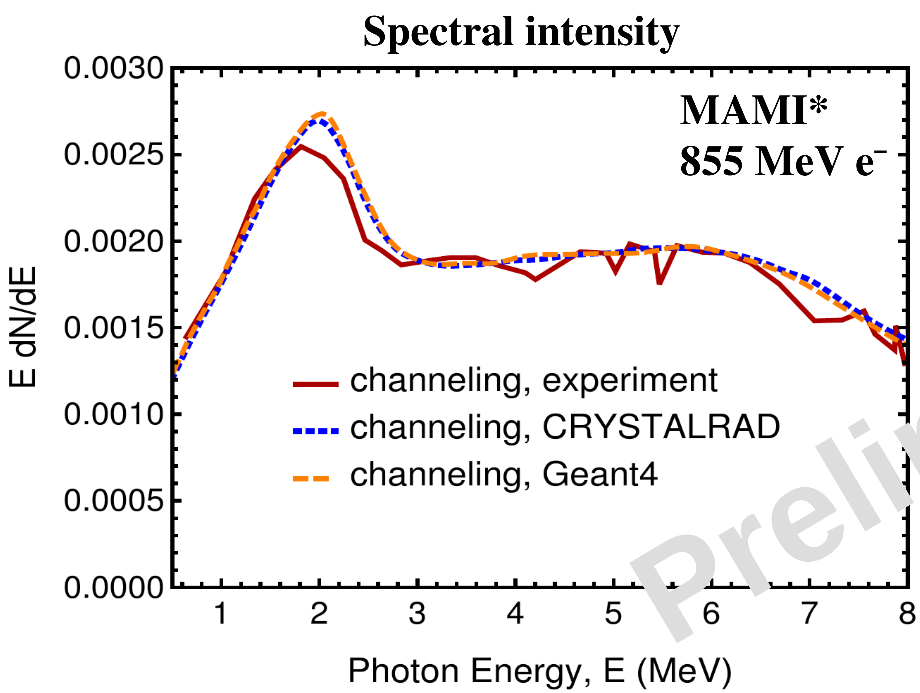
channeling

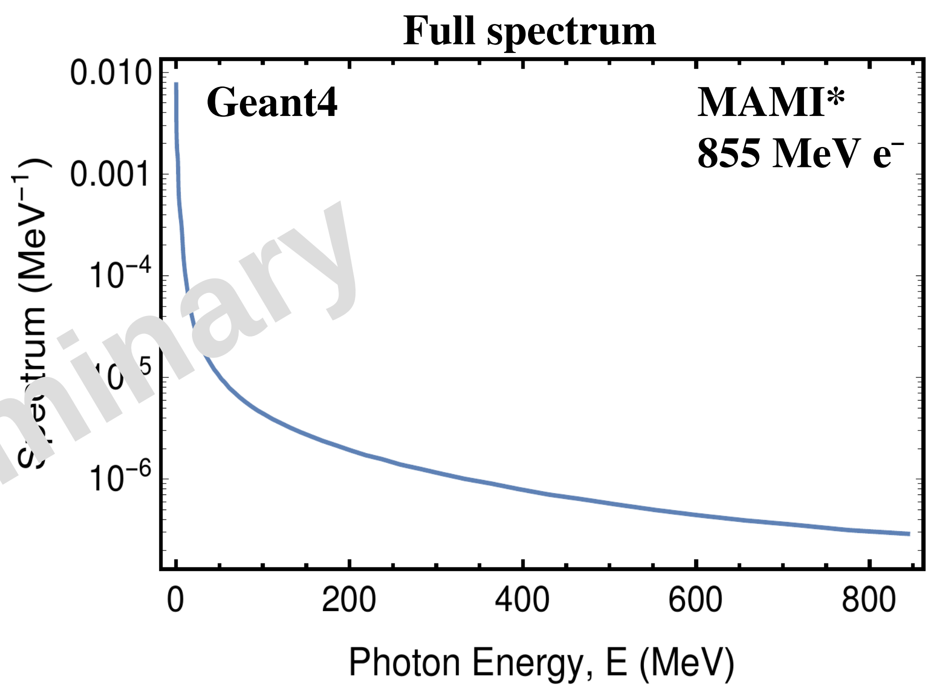
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

G4BaierKatkov:

- **Physics list independent**
- Can be used **outside channeling model** within other FastSim model
- Provides **radiation spectrum** for single-photon radiation mode
- Provides generation of **secondary photons**

Geant simulations vs experiment and CRYSTALRAD simulations



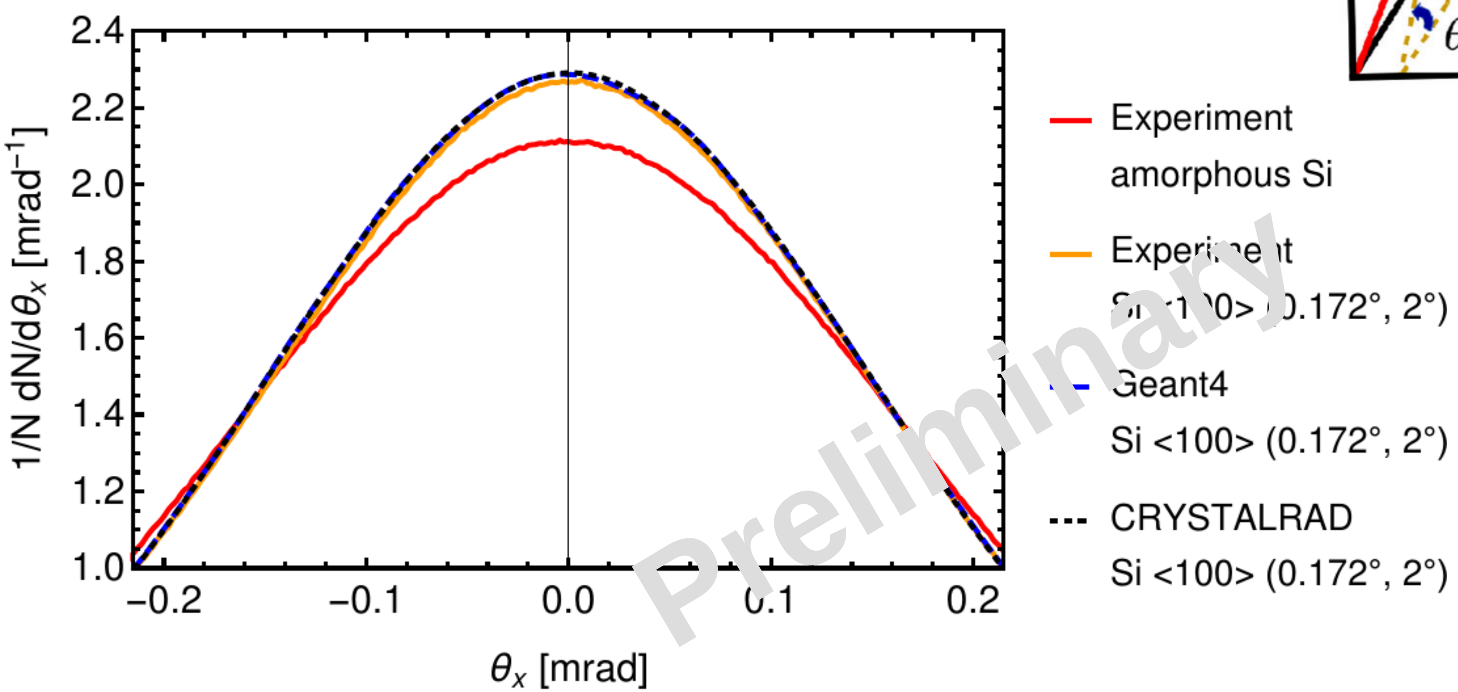


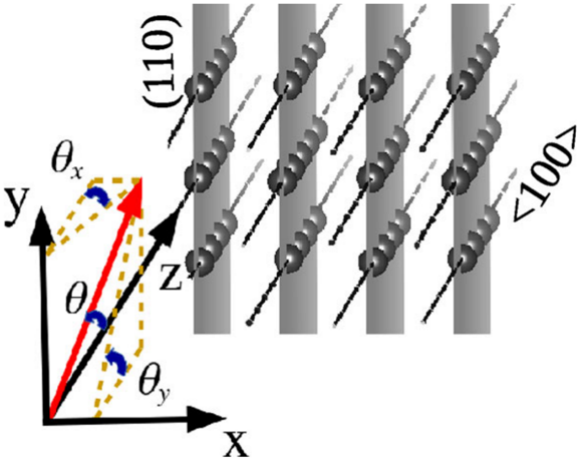
To be submitted for publication soon

*L. Bandiera et al. Phys. Rev. Lett. 115, 025504 (2015)

2D Geant4 channeling model validation: coherent scattering suppression effect*

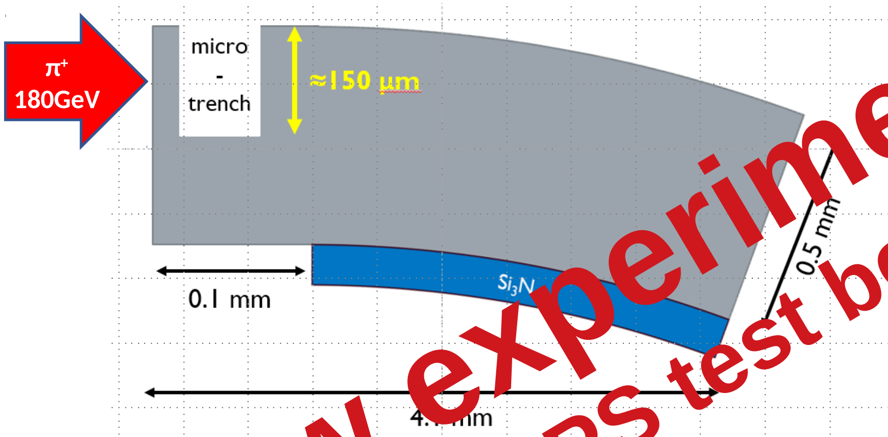
Multiple scattering in crystal and multiple scattering in amorphous material are different!



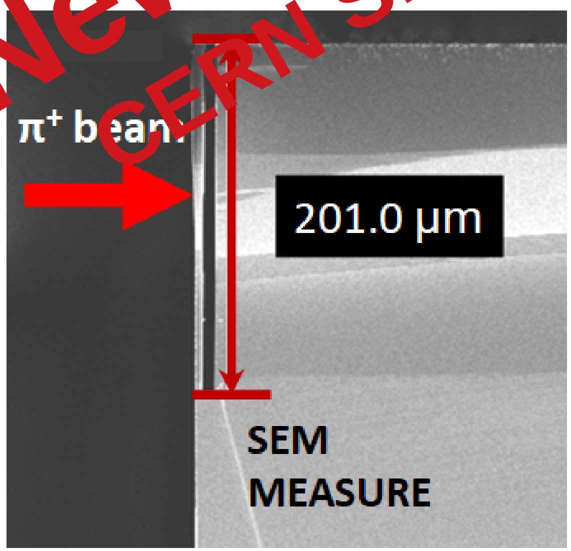


To be submitted for publication soon

Geant4 simulations of the experiment GALORE (2023): Crystalline cut to drastically increase the channeling efficiency



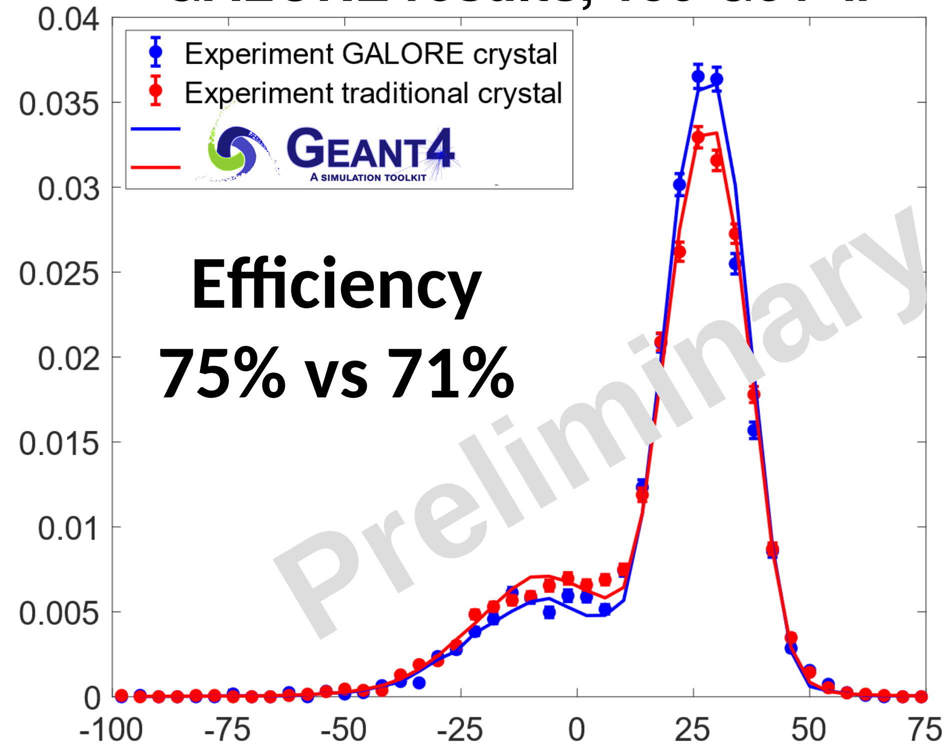
New experiment
CERN SPS test beam



Geant4 simulations vs experimental data

Courtesy of M. Romagnoni

GALORE results, 180 GeV π^+



M. Romagnoni, ..., A. Sytov et al. Crystals 12 (9), 1263 (2022)
M. Romagnoni, ..., A. Sytov et al. Eur. Phys. J. D 76, 135 (2022).

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

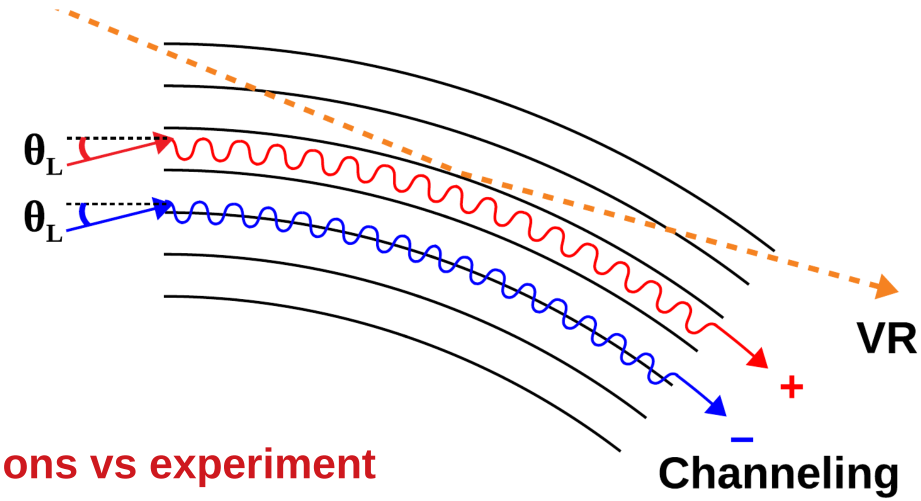
Recent experiment (March 2024)
Channeling of 530 MeV positrons in a bent crystal

MAINZER MIKROTRON

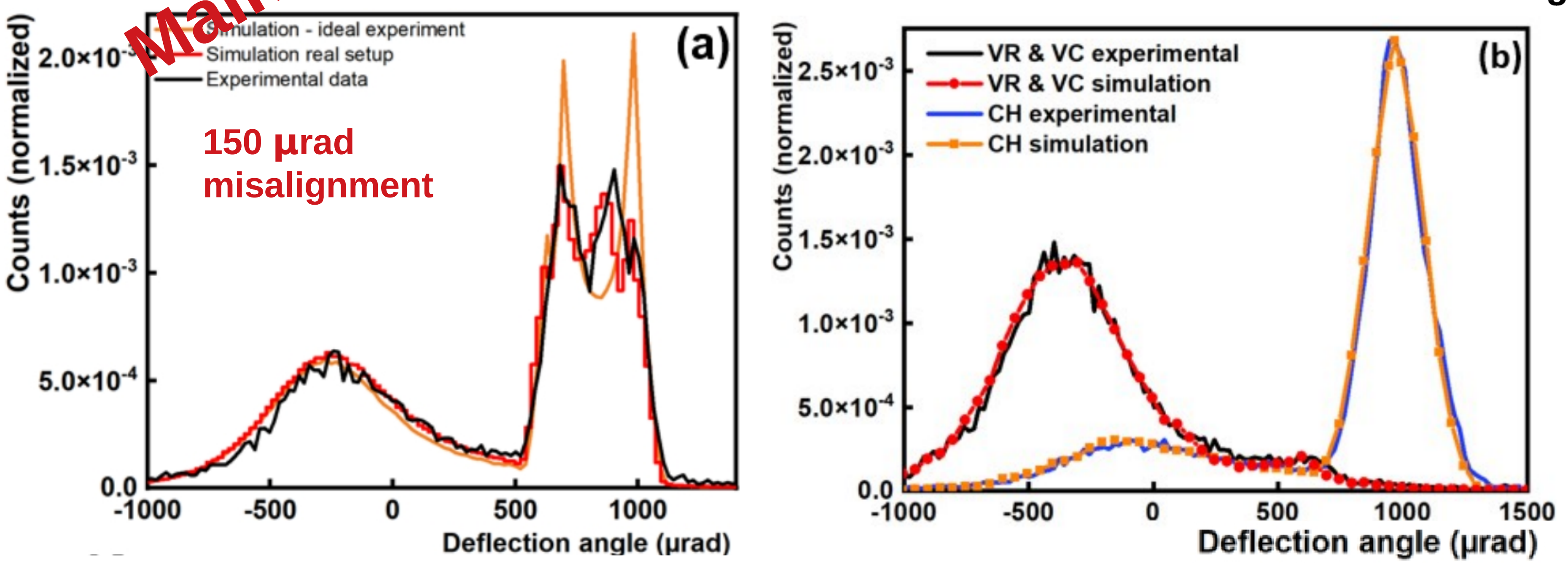
530 MeV positrons

30 µm thick bent crystal

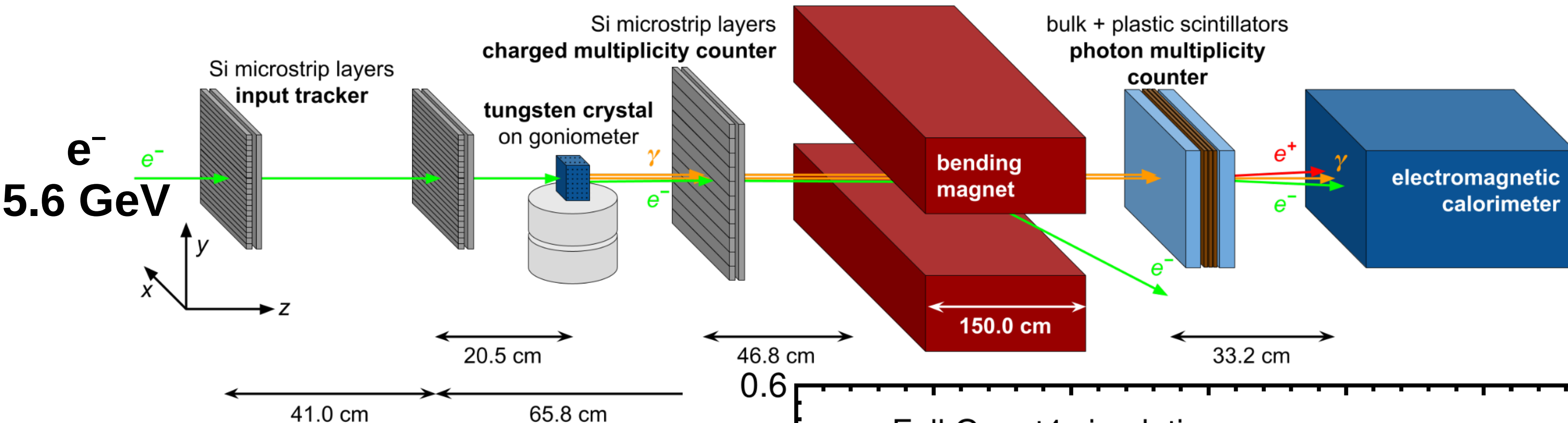
New experiment
Mainz Mikrotron 2024



Geant simulations vs experiment

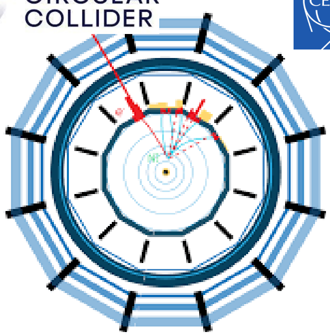


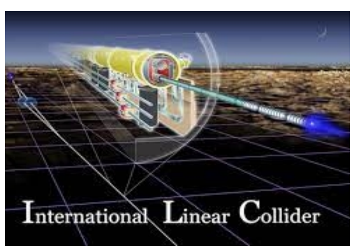
Full Geant4 simulations of the DESY experiment* for the FCC-ee positron source project

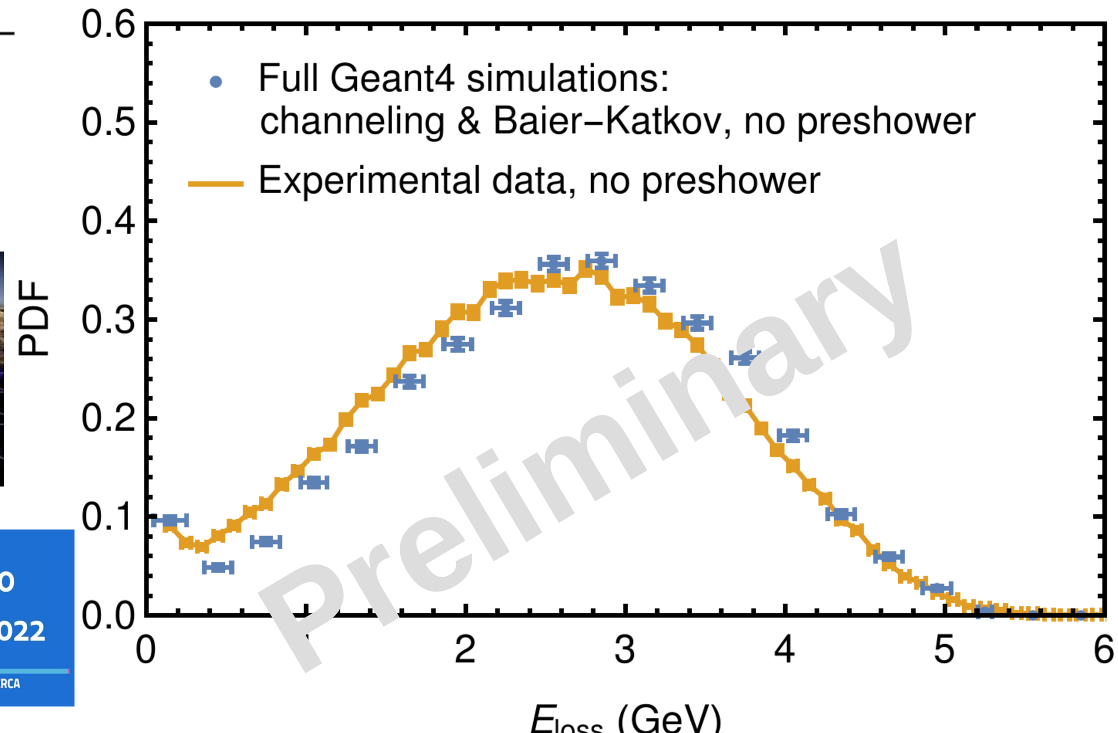


FUTURE CIRCULAR COLLIDER

CERN

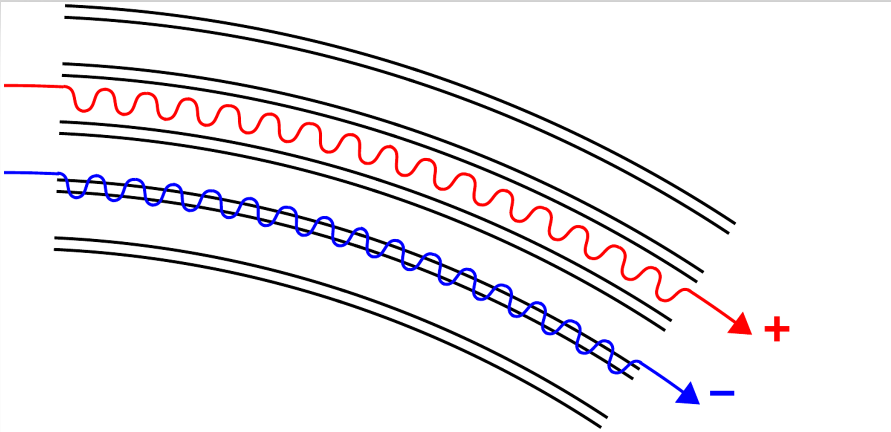






Intense positron source Based On Oriented cryST̲als - e+BOOST
(PI L. Bandiera)
PRIN2022-2022Y87K7X
Financed by Italian Ministry of University and Research - PRIN project

Crystal-based extraction

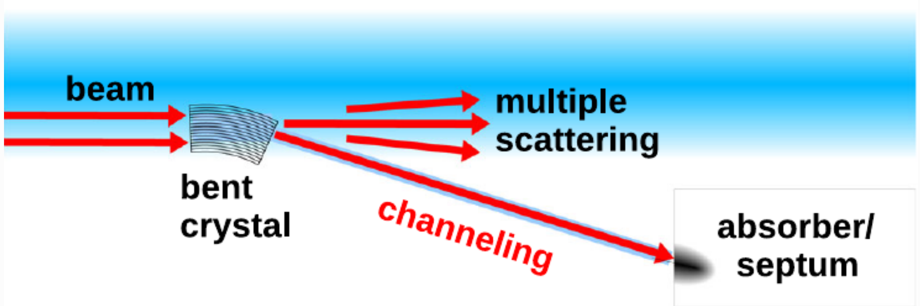


Channeling

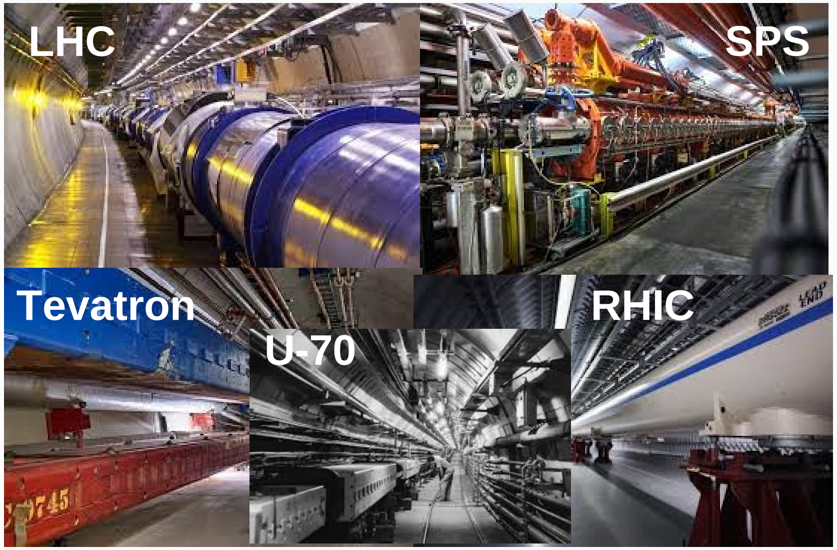
Planar channeling*:

- Charge particle penetration through a monocrystal along its atomic planes

Crystal-based extraction/collimation



Crystal-based collimation and **extraction have been used at hadron machines**



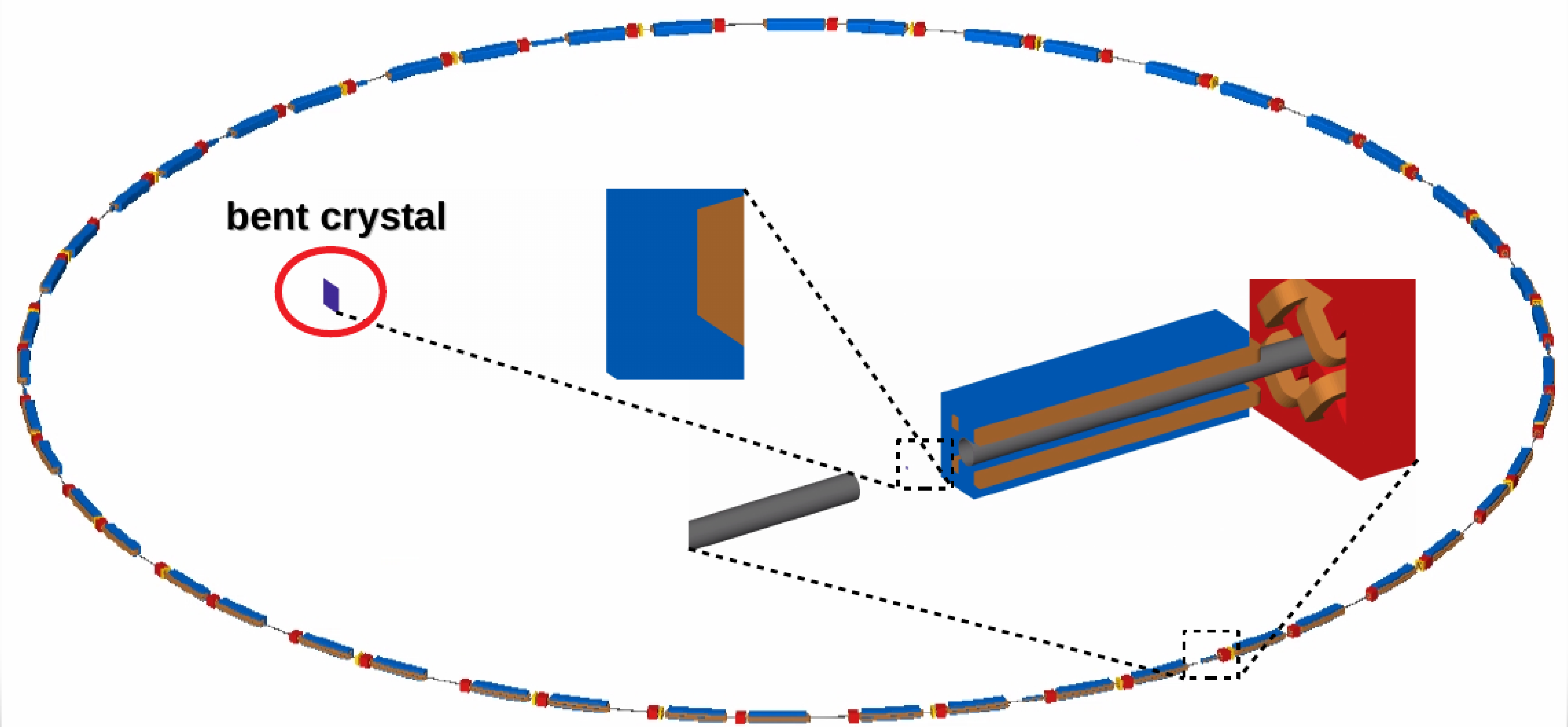
Crystal-based extraction/collimation: applied only for hadrons, not yet for e-

Interesting for tens of electron synchrotrons

***J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)**
E.N. Tsyganov, Fermilab TM-682 (1976)
A. Sytov et al. Eur. Phys. J. C 82, 197 (2022)

DESY-II Booster Synchrotron: full simulations with the BDSim simulation code

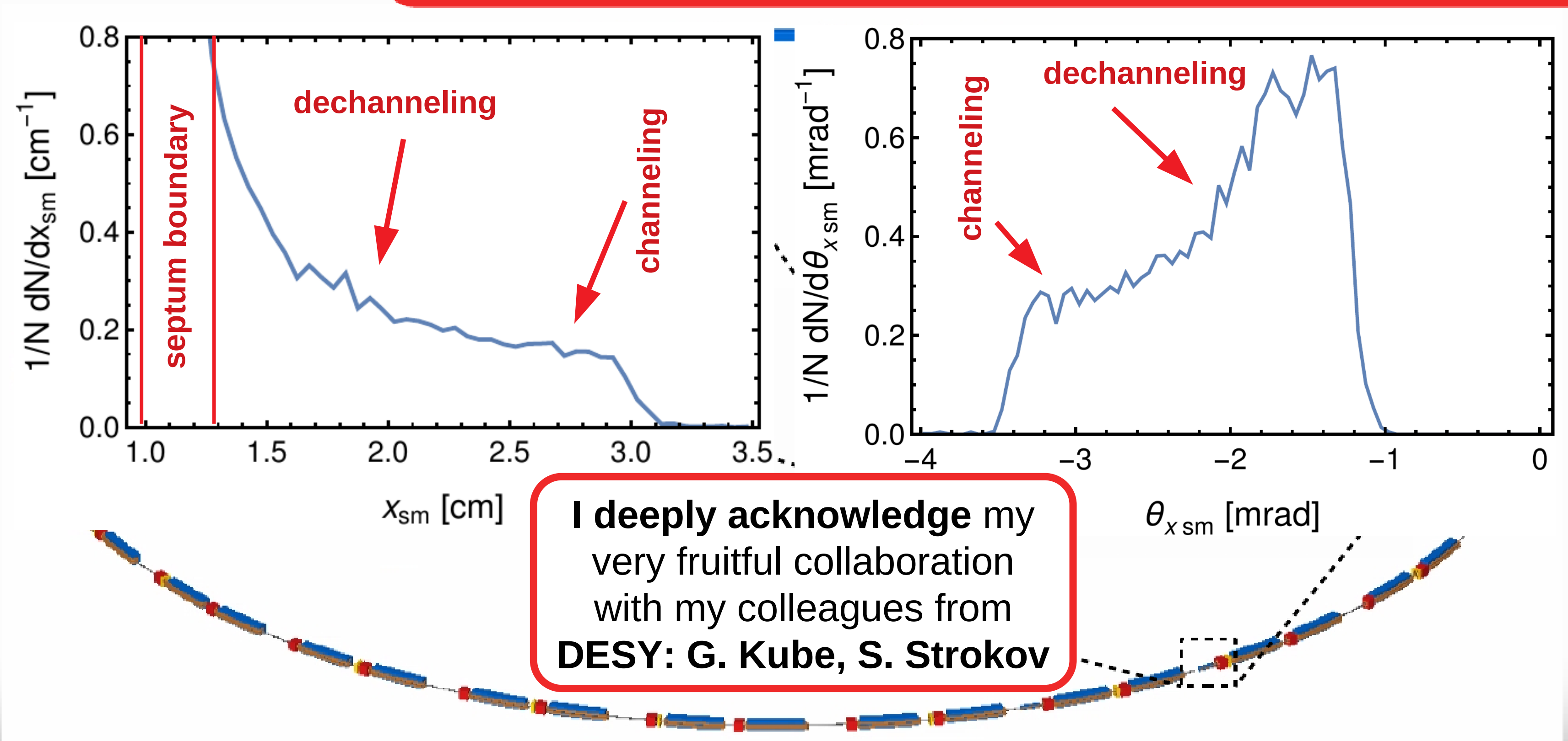
Purpose of BDSIM:
Beam Delivery Simulation (BDSIM) is a C++ program that utilises the **Geant4 toolkit** to simulate both the **transport of particles in an accelerator** and their **interaction with the accelerator material**. BDSIM is capable of **simulating a wide variety of accelerator components and magnets** with Geant4 geometry dynamically built based on a text input file. **Thick lens accelerator** tracking routines are provided for fast accurate tracking in a vacuum.



DESY-II Booster Synchrotron: full simulations with the BDSim simulation code

BDSIM
Beam Delivery Simulation

Purpose of BDSIM:
Beam Delivery Simulation (BDSIM) is a C++ program that utilises the **Geant4 toolkit** to simulate both the **transport of particles in an accelerator** and their **interaction with the accelerator material**. BDSIM is capable of **simulating a wide variety of accelerator components and magnets** with Geant4 geometry dynamically built based on a text input file. **Thick lens accelerator** tracking routines are provided for fast accurate tracking in a vacuum.



I deeply acknowledge my very fruitful collaboration with my colleagues from **DESY: G. Kube, S. Strokov**

Approximate list of examples to include in Geant4 in 2024

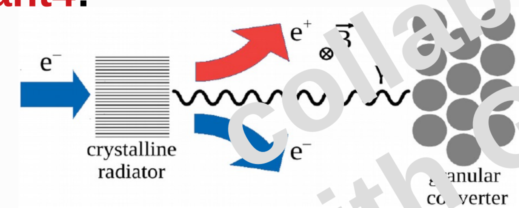
Probable updates of the channeling model: new model of ionization losses

Examples:

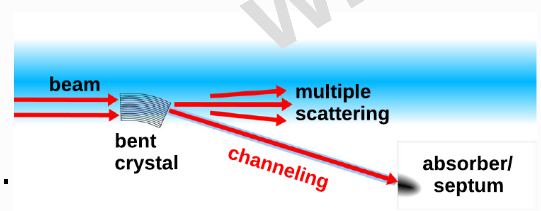
- Very **easy example** to demonstrate basic commands to include the channeling model in DetectorConstruction (no input/output) — **In test folder**
- **Complex example** including both channeling and radiation model, input with macro commands, root output and full spectrum of options — **Almost ready**
- **Pair production model** and dedicated example of electromagnetic shower in a scintillator crystal — **In development**

Specific applications to implement into Geant4:

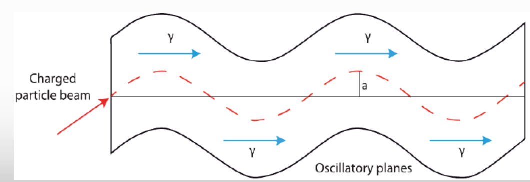
- **Crystal-based hybrid positron source for FCC-ee** — **Almost ready**



- **Crystalline deflector to extract a charged particle beam from an accelerator** (electron synchrotron, hadron collider) using **BDSim** code. — **Works! Needs to be finalized**



- **Crystalline undulator** — **Model exists in Geant4 kernel but needs to be validated**

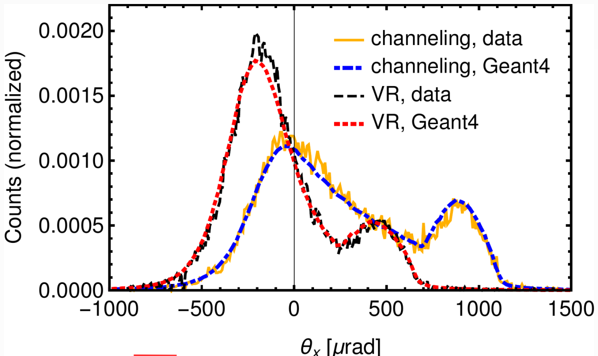


In close collaboration with G. Paternò

What's next? My proposal concerning neural networks

Geant4 simulations can produce **datasets** for **neural nets training.**
Neural nets are less precise but **much faster**!

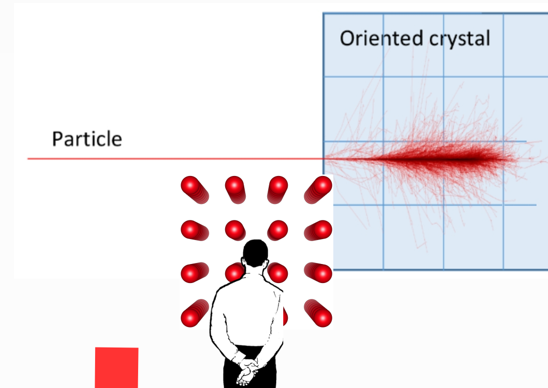
Step 1: beam deflection




```
Layer (type)                 Output Shape              Param #
=================================================================
dense (Dense)                (None, 200)               800

dense_1 (Dense)              (None, 500)               100500

dense_2 (Dense)              (None, 1000)              501000

dense_3 (Dense)              (None, 500)               500500

dense_4 (Dense)              (None, 200)               100200

dense_5 (Dense)              (None, 100)               20100
=================================================================
Total params: 1,223,100
Trainable params: 1,223,100
Non-trainable params: 0
```

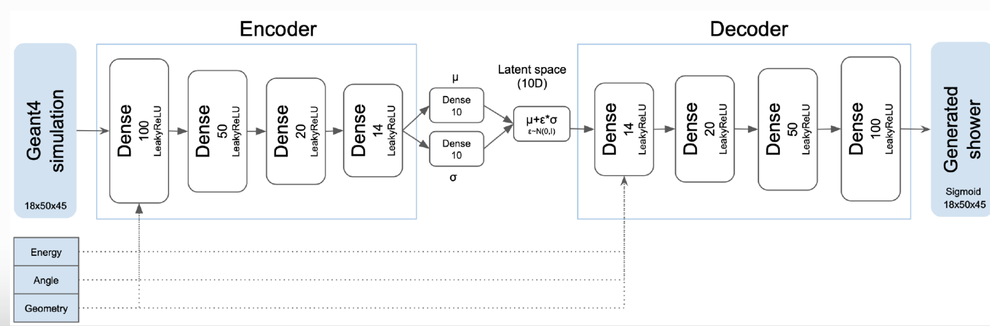
My first attempt

Step 2: electro magnetic shower



KISTI
www.kisti.re.kr
Korea Institute of Science and Technology Information

To use the **variational autoencoder** model already existing in **Geant4**
Anna Zaborowska & Marc Verderi



A modeling of the **full beamline** using **Geant4** is **required** for collimator design.

Dataset and **first ML** model generated **by PALLAS**

INFN Ferrara: implementation of plasma acceleration **ML model into Geant4** to create a **Geant4 electron beam source** based on plasma acceleration

```
#ifndef B1PrimaryGeneratorAction_h
#define B1PrimaryGeneratorAction_h 1

#include "G4VUserPrimaryGeneratorAction.hh"
#include "globals.hh"
#include "G4GeneralParticleSource.hh"
#include "G4ParticleGun.hh"
#include <memory>
#include <onnxruntime_c_api.h>
#include <onnxruntime_cxx_api.h>
class G4ParticleGun;
class G4Event;
```

```
PrimaryGeneratorAction::PrimaryGeneratorAction(): G4VUserPrimaryGeneratorAction(),
    fParticleGun(0),
    fEnvelopeBox(0)
{
    G4int n_particle = 1;
    fParticleGun  = new G4ParticleGun(n_particle);

    // default particle kinematic
    fParticleGun->SetParticleDefinition(
        G4ParticleTable::GetParticleTable()->FindParticle("e-"));

    //Neural network: create onnx session
    Ort::Env env(ORT_LOGGING_LEVEL_WARNING, "plasma");
    Ort::SessionOptions session_options;
    session_options.SetIntraOpNumThreads(1);
    auto sessionLocal =
        std::make_unique<Ort::Session>(env, "model2.onnx", session_options);
    fSession = std::move(sessionLocal);

    // Get input node information
    fMemory_info = Ort::MemoryInfo::CreateCpu(
        OrtAllocatorType::OrtArenaAllocator, OrtMemTypeDefault);
```

Publications

TRILLION publications:

- A. Sytov et al. Journal of the Korean Physical Society 83, 132-139, (2023). DOI: https://doi.org/10.1007/s40042-023-00834-6 arXiv:2303.04385
- L. Bandiera, ..., A. Sytov, et al. Eur. Phys. J. C 82, 699 (2022). DOI: https://doi.org/10.1140/epjc/s10052-022-10666-6
- A. Sytov et al. Eur. Phys. J. C 82, 197 (2022). DOI: https://doi.org/10.1140/epjc/s10052-022-10115-4
- M. Romagnoni, ..., A. Sytov et al. Crystals 12 (9), 1263 (2022). DOI: https://doi.org/10.3390/cryst12091263
- M. Romagnoni, ..., A. Sytov et al. Eur. Phys. J. D 76, 135 (2022). DOI: https://doi.org/10.1140/epjd/s10053-022-00439-x
- M. Soldani, …, A. Sytov et al. Eur. Phys. J. C 83, 101 (2023). DOI: https://doi.org/10.1140/epjc/s10052-023-11247-x
- L. Bandiera, …, A. Sytov et al. Frontiers in Physics 11 Pages: 1254020 (1-11) (2023). DOI: https://doi.org/10.3389/fphy.2023.1254020
- Max F. Gilljohann, …, A. Sytov et al. JINST 18, P11008 (2023) DOI: 10.1088/1748-0221/18/11/P11008 arXiv:2203.07459
- K. Park, K. Kim, A. Sytov, K. Cho. J. Astron. Space Sci. 40 (4), 259-266 (2023). DOI: https://doi.org/10.5140/JASS.2023.40.4.259
- M. Soldani, …, A. Sytov et al. Nuclear Instruments and Methods in Physics Research, Section A 1058, 168828 (1-6) (2024) DOI: https://doi.org/10.1016/j.nima.2023.168828
- L. Bandiera, …, A. Sytov et al. Nuclear Instruments and Methods in Physics Research, Section A 1060, 169022 (2024). DOI: https://doi.org/10.1016/j.nima.2023.169022
- K. Park, K. Kim, A. Sytov, K. Cho. Journal of the Korean Physical Society, 84, 403–426, (2024). DOI: https://doi.org/10.1007/s40042-024-01005-x
- A. Mazzolari ,…, A. Sytov et al. arXiv:2404.08459 submitted to PRL


GANGNAM STYLE
Thank you! 감사합니다 !