Geant4 ab-initio models on channeling, channeling radiation and coherent pair production in oriented crystals

Marie Curie Global Fellowships, Project TRILLION GA n. 101032975

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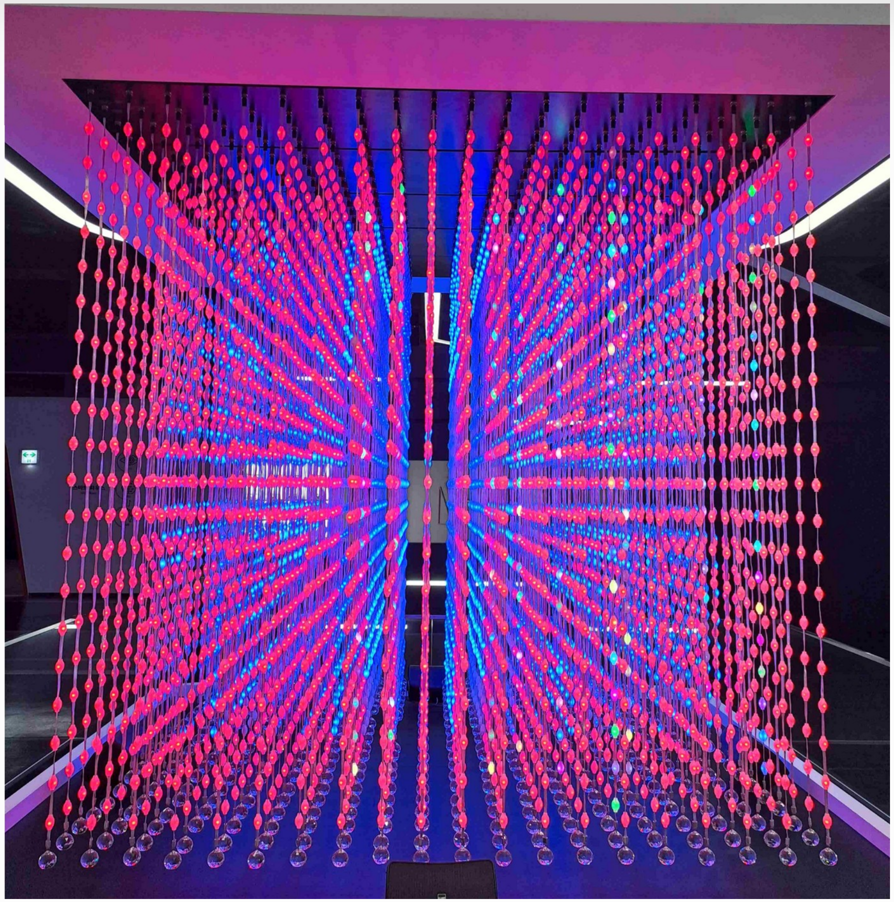
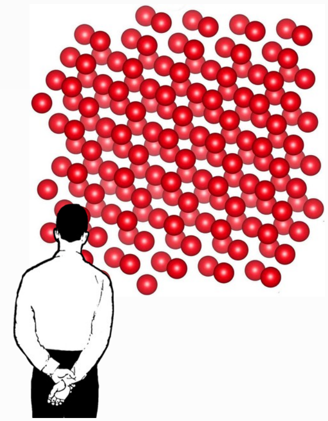
29th Geant4 Collaboration Meeting, 10/10/2024

How an oriented crystal looks like

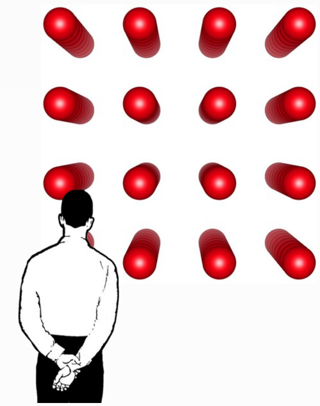


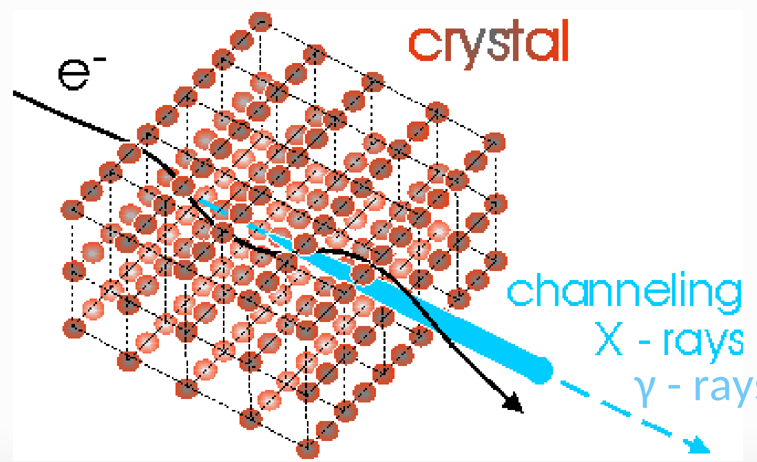
from National Science Museum, Daejeon, Korea

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:

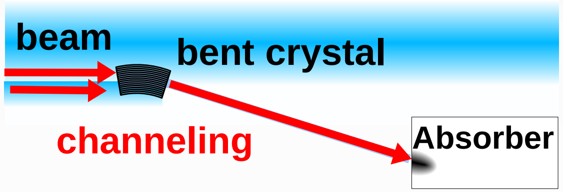
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

Location:

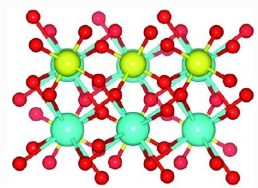
- 2 years at **KISTI** (partner organization)
- 1 year at **INFN Section of Ferrara** (host organization)
- 1 month of secondment at **DESY** (partner organization)
- 1 month of secondment at **IJCLab Orsay** (partner organization)

Applications*

Crystal-based collimation or beam extraction from an accelerator

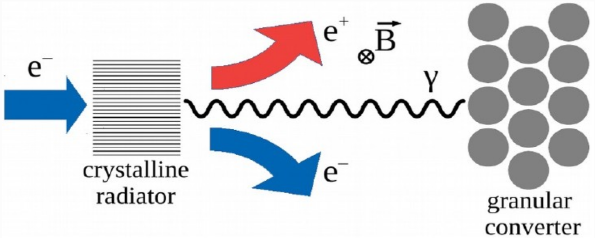


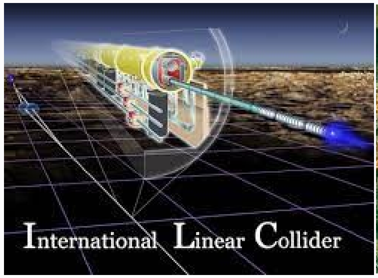
Ultrashort crystalline calorimeter

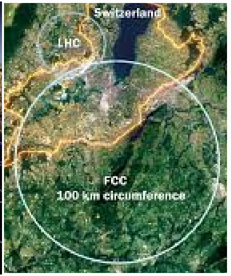


Gamma-ray Space Telescope

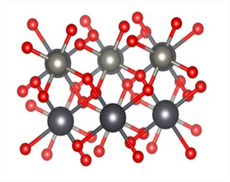
Positron source for future e+/e- and muon colliders



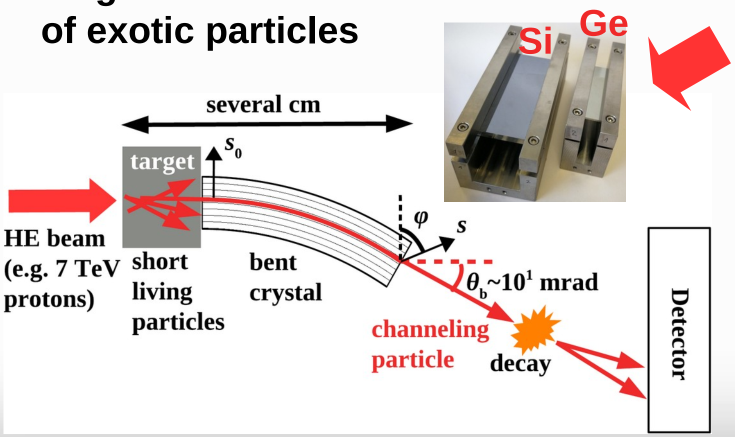




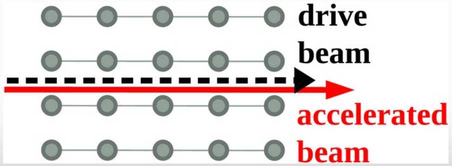
Oriented crystals



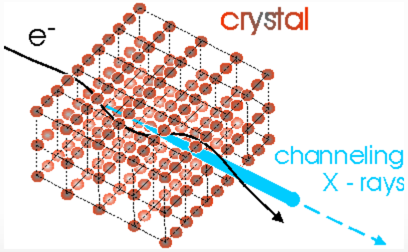
Measurement of dipole magnetic and electric moments of exotic particles

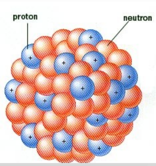


Plasma acceleration



X and γ-ray source for nuclear and medical physics



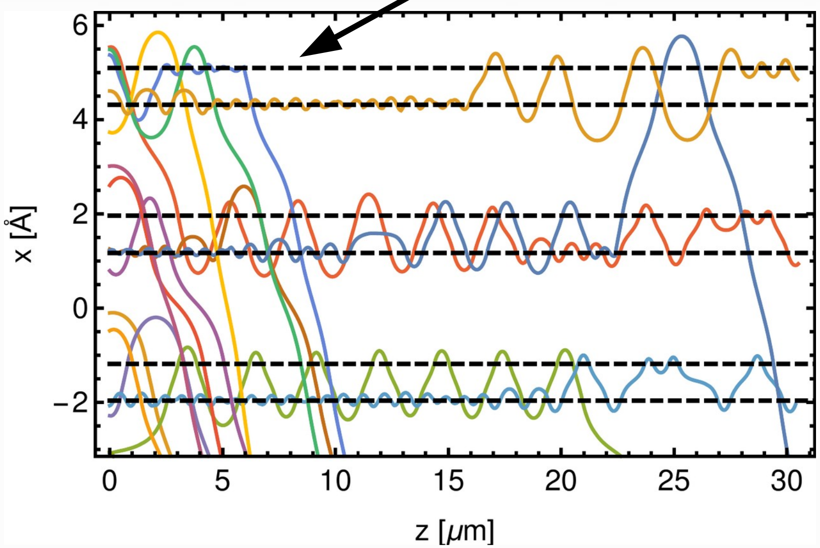


*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

G4ChannelingFastSimModel and G4BaierKatkov

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

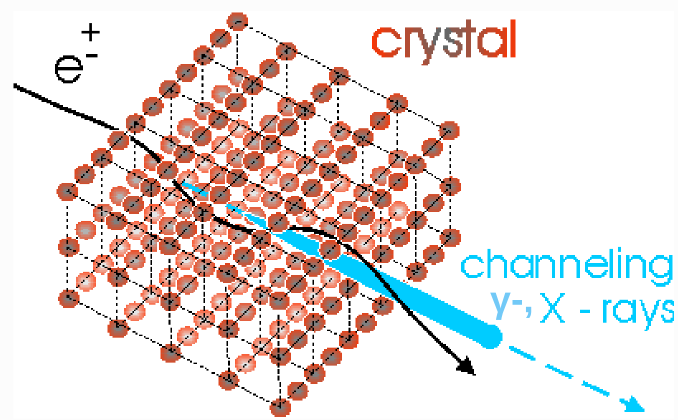


channeling*

New 2024: ionization losses in channeling

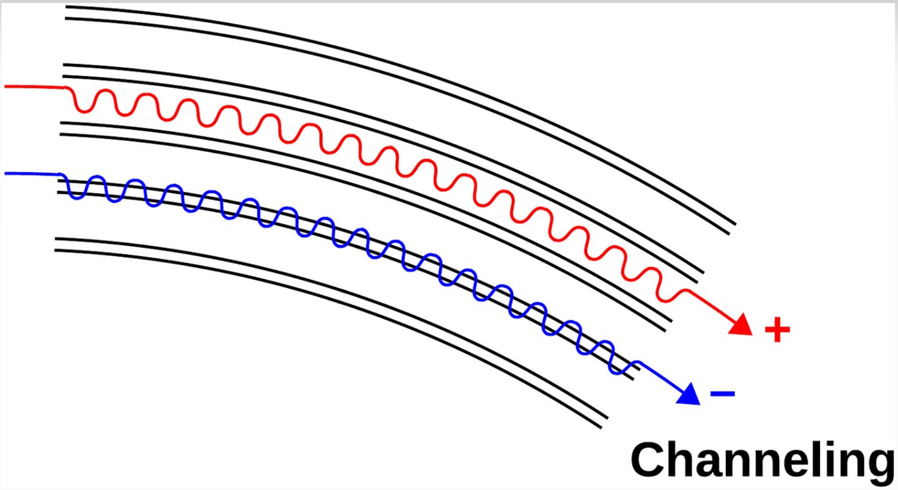
Baier-Katkov formula:
integration is made over the classical trajectory

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



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

Channeling



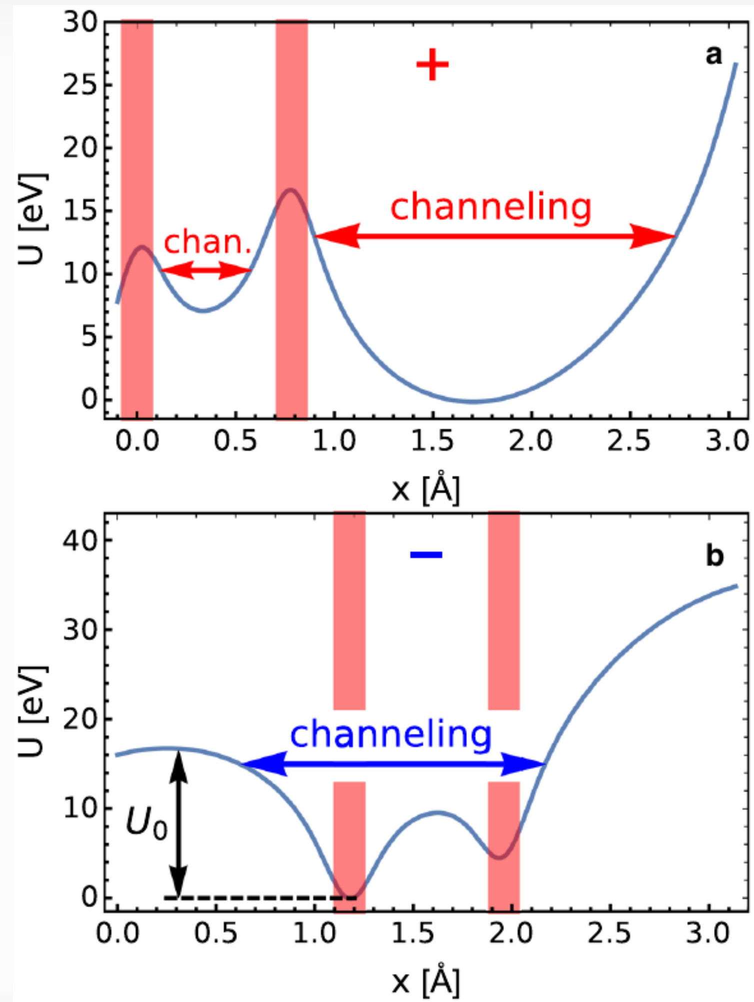
Channeling*:

Charge particle penetration through a monocrystal along its atomic planes/axes

trajectory equation:

$$\frac{d^2x}{dz^2} + \frac{U'_{pl\ x}}{pv} + \frac{1}{R} = 0$$

Interplanar potential



***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 (2022) 82:197**

The model of Coulomb scattering

Coulomb scattering cross-section on atom following from screened Coulomb potential:

$$\frac{d\sigma_{cr}}{d\Omega} = \frac{d\sigma_{coh}}{d\Omega} + \frac{d\sigma_{inc}}{d\Omega} \qquad \frac{d\sigma_{inc}}{d\Omega} = N(1-D)\frac{d\sigma_{at}}{d\Omega}$$

Motion in averaged potential

Debye-Waller factor

Coulomb scattering process is divided into **multiple** and **single scattering**:

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

$$<\vartheta^2_{Cms}> = <n_N> \Delta z \int_0^{\vartheta_2}\int_0^{2\pi} \frac{d\sigma_C}{d\Omega}\left(1-\exp(-p^2\vartheta^2 u_1^2)\right) d\varphi \vartheta^3 d\vartheta$$

Debye-Waller factor

- **Single scattering** $\vartheta > \vartheta_2$ by **(1)** and taking into account the **Debye-Waller factor**.
- **Single scattering on electrons**, Rutherford cross-section:

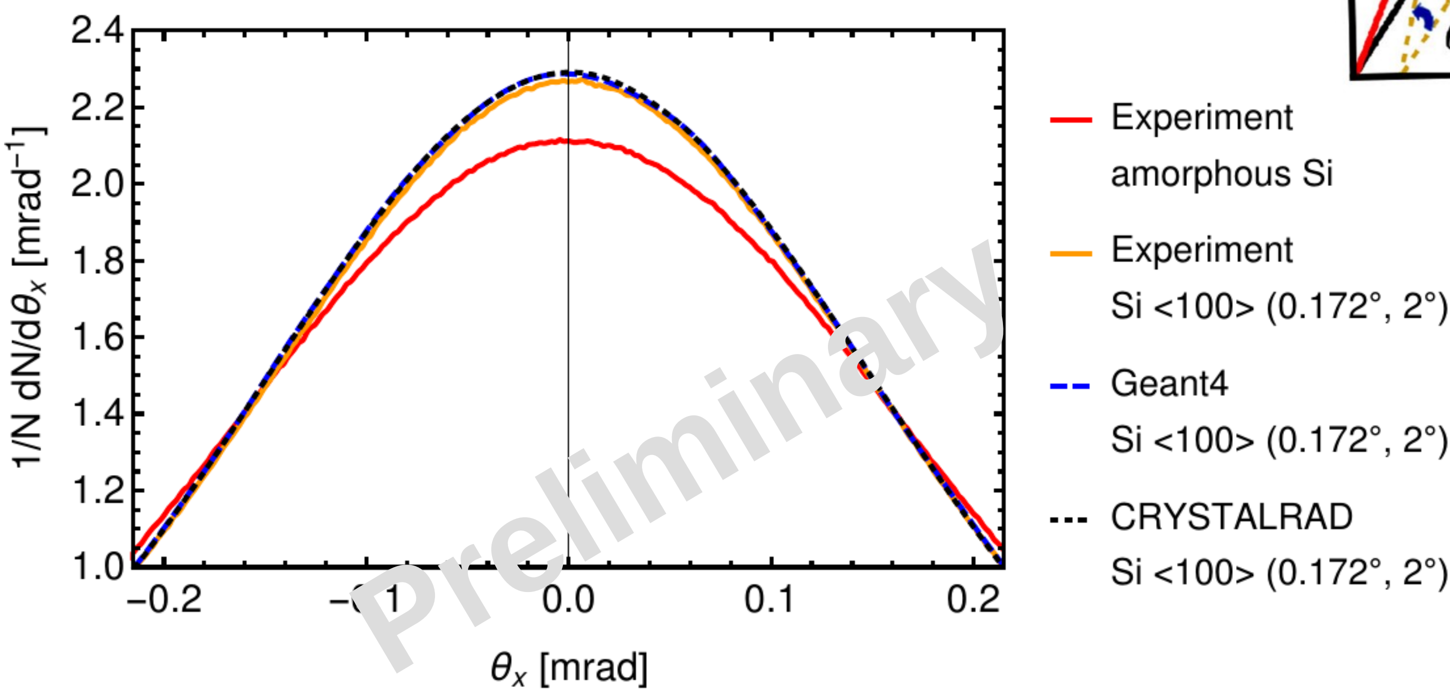
$$\frac{d\sigma_{Ce}}{d\Omega} = 4\frac{z^2 e^4}{p^2 v^2}\frac{1}{\vartheta^4}$$

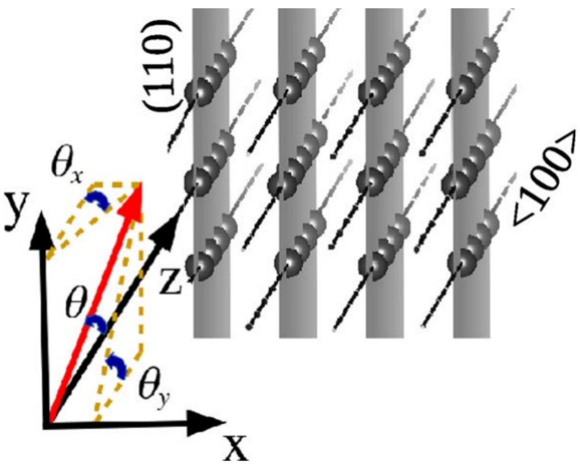
M. L. Ter-Mikaelian, High-energy electromagnetic processes in condensed media. Wiley. New York, 1972.

A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

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

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



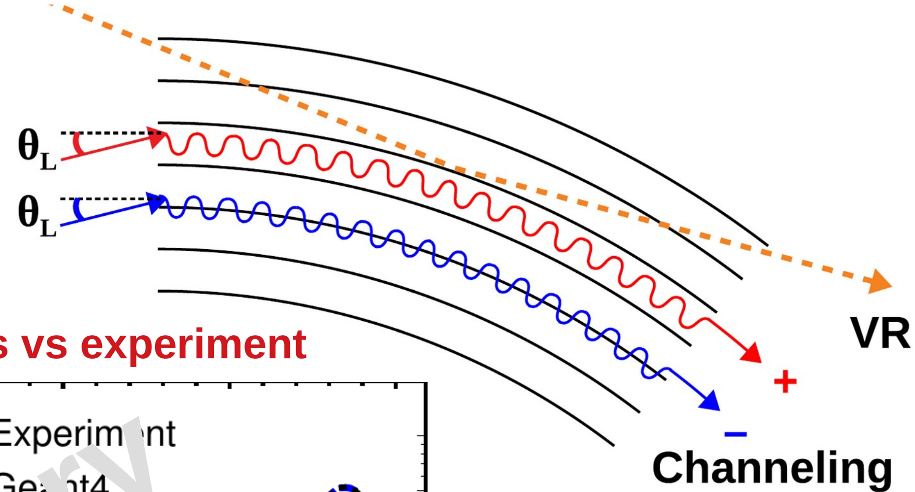


To be submitted for publication soon

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

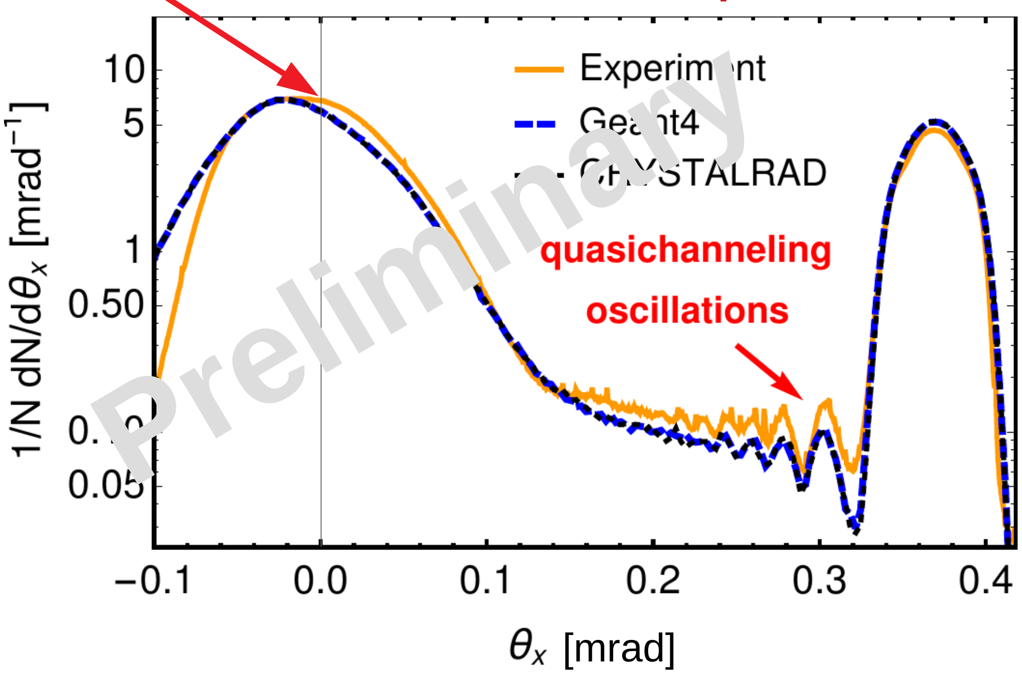
20.35 GeV positrons

60 µm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



channeling

To be submitted for publication soon

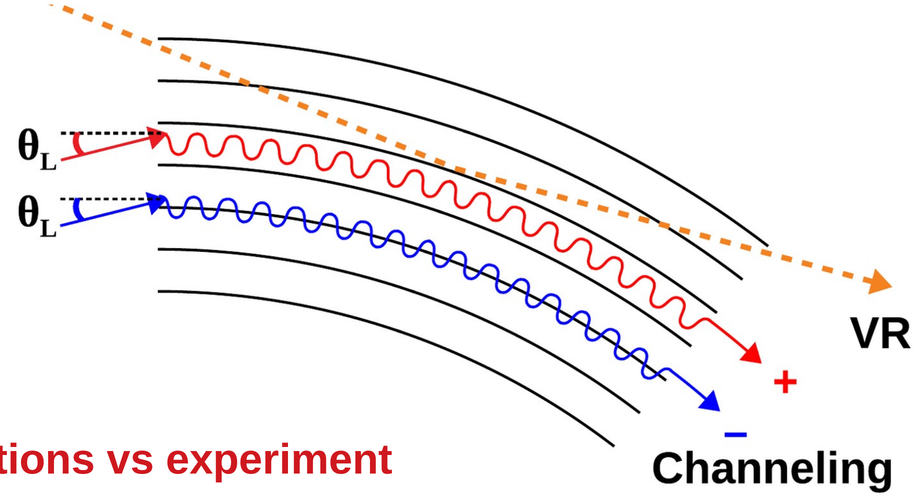
*T. N. Wistisen, …, and A. Sytov, Phys. Rev. Lett. 119, 024801 (2017)

Recent experiment
Channeling of 530 MeV positrons in a bent crystal

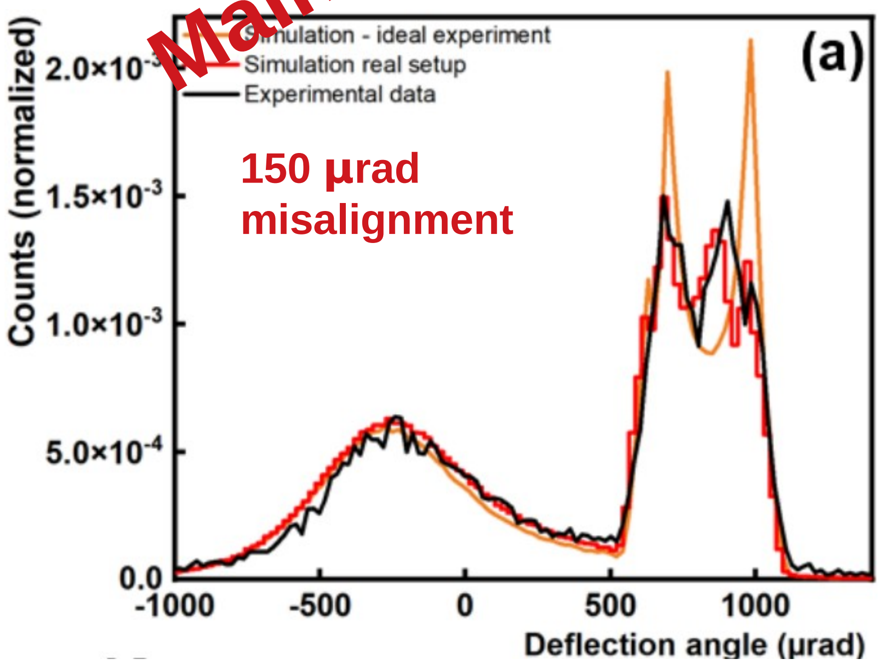
530 MeV positrons

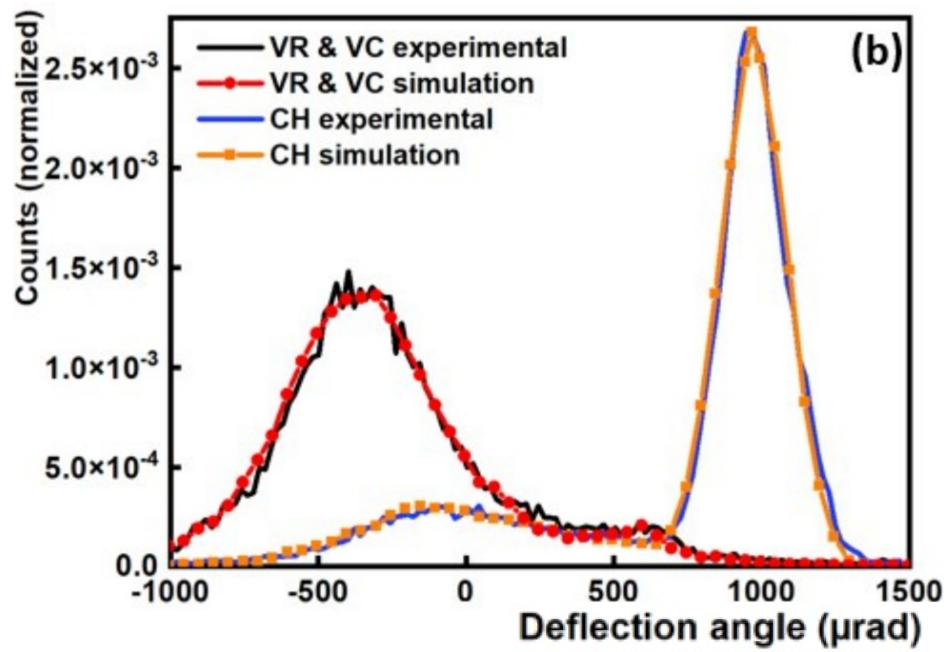
30 µm thick bent crystal

New experiment Mainz Mikrotron 2024



Geant4 simulations vs experiment





Main concept of full ab-inition G4BaierKatkov

$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{[(E^2+E'^2)(v_1v_2-1)+\omega^2/\gamma^2]}{2E'^2} e^{-ik'(x_1-x_2)}$$

Monte Carlo integration by photon **3 components of momentum**

$\vec{k}$

Monte Carlo integration by photon **energy** and **angles**

$\omega, \theta x, \theta y$

Radiation probability calculated **per photon**

$$\vec{k}_i \Rightarrow P_i$$

If radiation happens, **select a photon** from using ***Pi*** as their **weight** and generate it

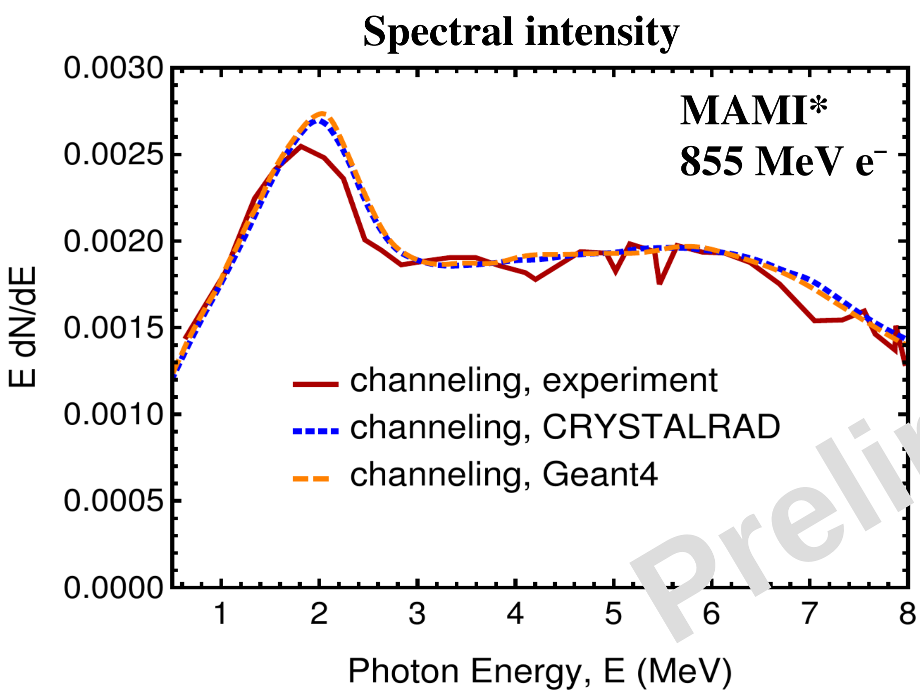
Photon **energy** and **angular distribution** naturally comes **from Baier-Katkov**

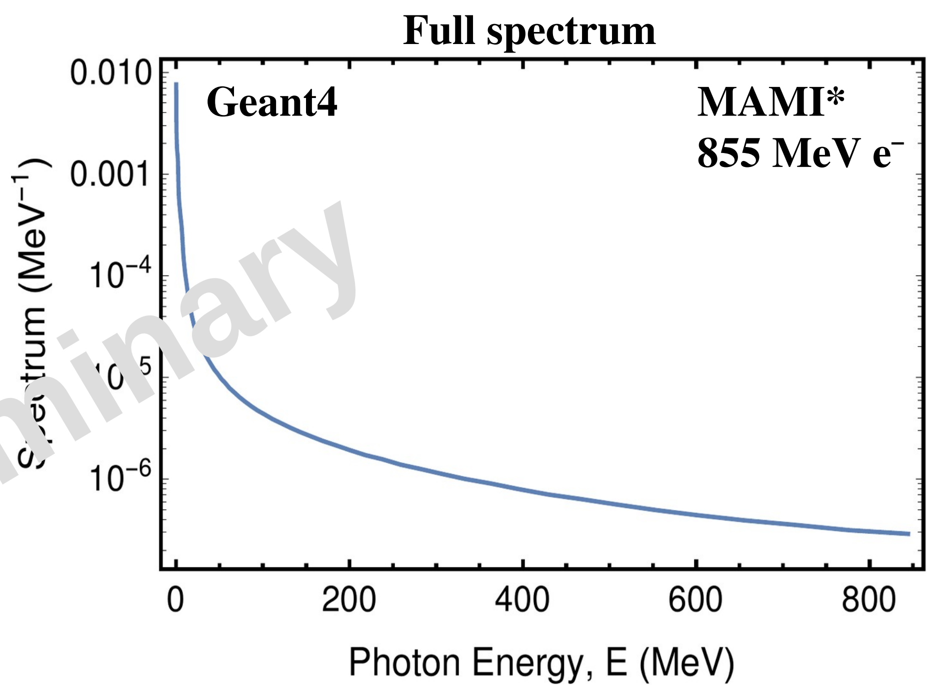
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

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)

How to implement an external code into Geant4?
Geant4 FastSim interface, solution to most of challenges

FastSim model:

- **Physics list independent**
- Declared in the **DetectorConstruction** (just **few lines of code**)
- Is activated **only** in a **certain G4Region** at a **certain condition** and only for **certain particles**
- **Stops Geant processes** at the step of FastSim model and then resumes them

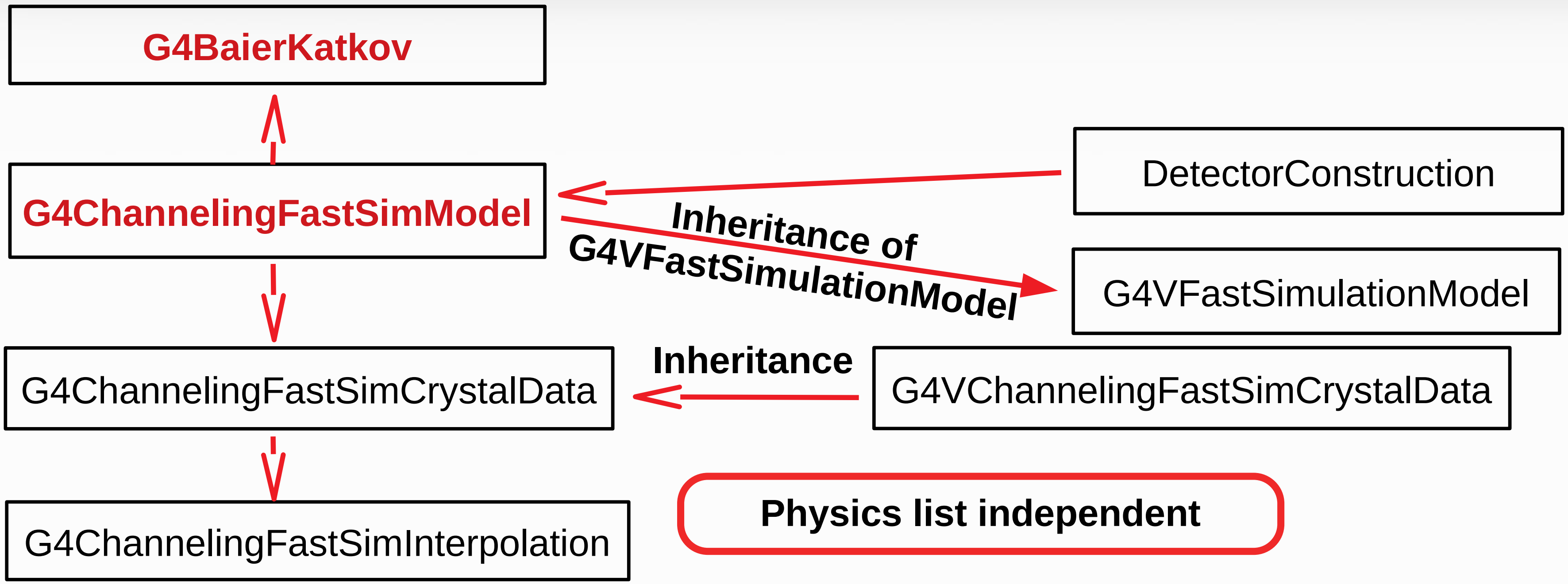
```
G4bool TestModel::IsApplicable(const G4ParticleDefinition& particleType)
{
  return
    &particleType == G4Proton::ProtonDefinition()||
    &particleType == G4AntiProton::AntiProtonDefinition()||
    &particleType == G4Electron::ElectronDefinition() ||
    &particleType == G4Positron::PositronDefinition();// ||
    //&particleType == G4Gamma::GammaDefinition();
}

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......

G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
{
}

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......

void TestModel::DoIt(const G4FastTrack& fastTrack,
                     G4FastStep& fastStep)
{
```

Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

Structure of classes



Additional classes:

- **G4VChannelingFastSimCrystalData:** multiple and single Coulomb scattering, ionization losses
- **G4ChannelingFastSimCrystalData:** read crystal lattice data files from **G4CHANNELINGDATA**, logical volume to crystal plane/axis geometry transformation
- **G4ChannelingFastSimInterpolation:** crystal lattice data and 3D-spline interpolation functions

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

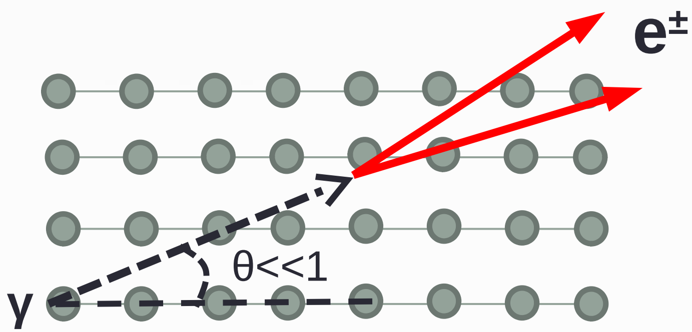
Geant4 Physics Reference Manual:

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)

Coherent pair production***



Key idea:

- Randomly **generate e± pairs**
- **Track e±** in the crystal
- Use **Baier-Katkov** formula to calculate the **probability of pair production**
- Randomly **select a pair according to this probability** and generate secondaries

G4CoherentPairProduction ← **G4CoherentPairProductionPhysics**

↓

G4ChannelingFastSimCrystalData ← (**Inheritance**) G4VChannelingFastSimCrystalData

↓

G4ChannelingFastSimInterpolation

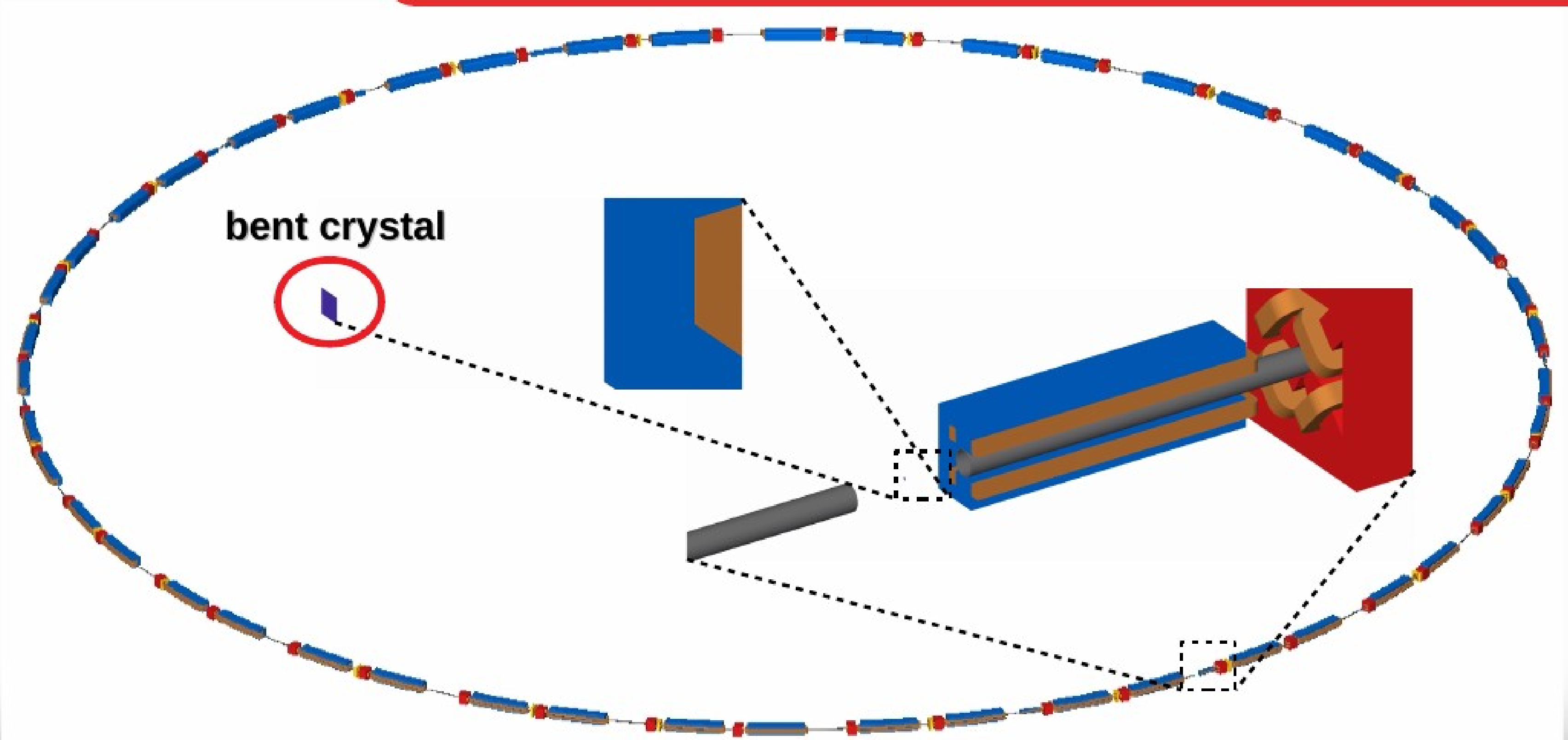
Can work in parallel with standard physics list

*** H. Überall, Phys. Rev. 103, 1055 (1956)

My mission to DESY:
full simulations with the BDSim simulation code

BDSIM
Beam Delivery Simulation

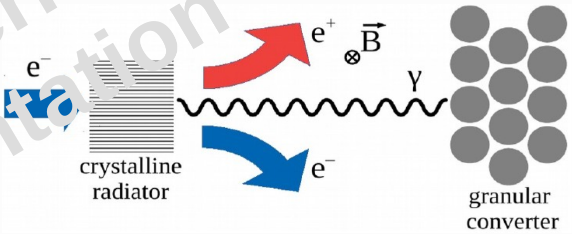
Purpose of BDSIM:
Beam Delivery Simulation (BDSIM) is a C++ program that utilises the **Geant4 toolkit** to simulate both the **transport of particles in an accelerator** and their **interaction with the accelerator material**. BDSIM is capable of **simulating a wide variety of accelerator components 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.



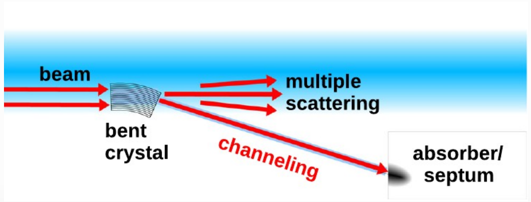
To include in Geant4 in 2024

Examples:

- **ch1** a very **easy example** to demonstrate basic commands to include the channeling model in DetectorConstruction (no input/simple output) — **Merged**
- **ch2** a **complex example** including both channeling and radiation model, crystalline undulator, input with macro commands, root output and full spectrum of options — **Merged**
- **Crystal-based hybrid positron source for FCC-ee** — **Prepared**



- **Pair production model** and dedicated example of electromagnetic shower in a scintillator crystal — **Model prepared; example in 2025**
- **Crystalline deflector to extract a charged particle beam from an accelerator** (electron synchrotron, hadron collider) using **BDSim** code — **Works**



Acknowledgments

Marie Sklodowska-Curie Action Global Individual Fellowships TRILLION (G.A. 101032975) is in synergy with the following projects I would like to acknowledge:

- **GEANT4INFN** project (INFN Geant4 group);
- **INFN OREO, PRIN E+BOOST, INFN GALORE, RD-MUCOL, RD-FCC,**
- **H2020-MSCA-RISE N-LIGHT** (G.A. 872196) and **EIC-PATHFINDER-OPEN TECHNO-CLS** (G.A. 101046458) projects.
- We acknowledge the **CINECA** award under the **ISCRA** initiative, for the availability of high-performance computing resources and support.
- This work is also supported by the Korean National Supercomputing Center with supercomputing resources including technical support (**KSC-2022-CHA-0003**).

I also thank the **Geant4 collaboration** members, in particular:

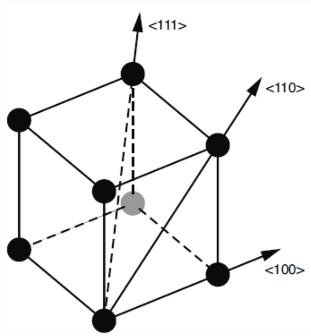
Prof. Vladimir Ivanchenko (**CERN**), **Prof. Pablo Cirrone and Dr. Luciano Pandola** (**INFN LNS**), **Prof. Kihyeon Cho, Prof. Soonwook Hwang** and **Dr. Kyungho Kim** (**KISTI**), **Prof. Susanna Guatelli** and **Prof. Anatoly Rosenfeld** (**University of Wollongong**), **Dr. Gianfranco Paternò (INFN Ferrara) as well as Prof. Makoto Asai (Jlab) and Prof. Marc Verderi (IN2P3/LLR)** for fruitful collaboration and discussions!

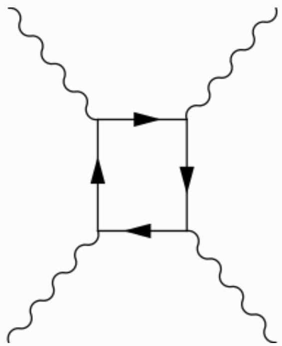

GANGNAM STYLE
감사합니다 !

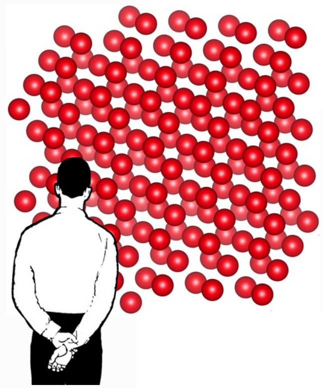
Electromagnetic shower acceleration

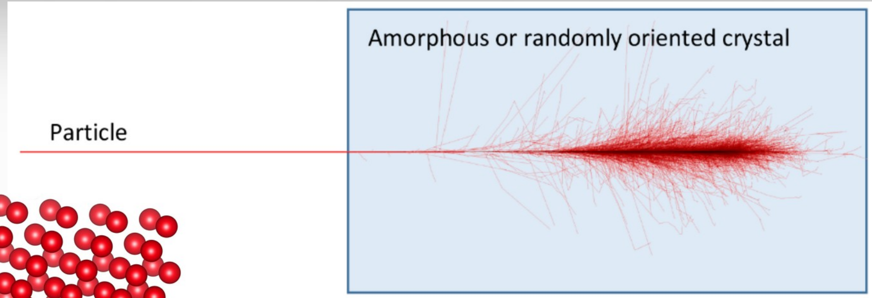
Axial field 10^{11} V/cm

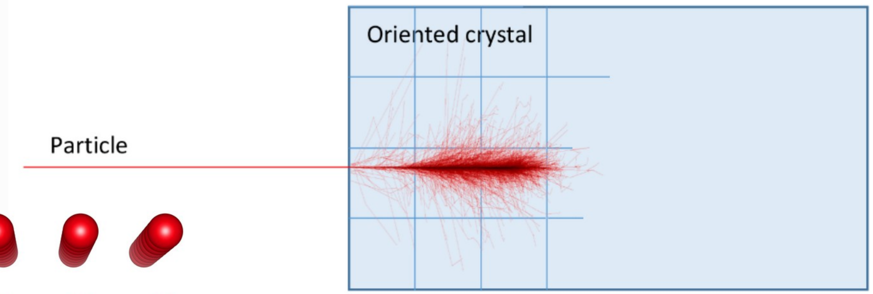
Approaching the **Schwinger limit** starting from few **GeV** for **e+/e-**

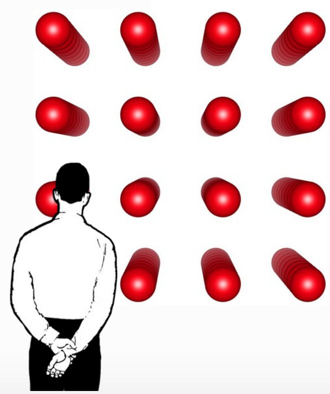












The **radiation** intensity and the **pair production** cross-section **drastically increase** in **oriented crystals!**

Shower development in the field of axes is **accelerated**. The radiation length is considerably reduced.

Why the implementation of channeling and Baier-Katkov models into Geant4 is so challenging?

Challenges of trajectory simulation

- **Complicated geometry** of crystal planes/axes especially in a bent crystal;
- **Complicated spacial structure** of cristalline **electric fields** and **atomic density** depending on the material and alignment;
- Different types of **scattering dependent** on the charge particle **positions** vs crystal planes/axes;
- **Incompatibility** of channeling with **Geant4 standard physics lists**: especially with **multiple coulomb scattering** and **bremsstrahlung** process: impossible to modify **continuous-discrete Geant4** processes during execution.

Challenges of Baier-Katkov

- Need for **recording trajectory** in order to simulate the spectrum;
- Multidimensional integral => **low simulation speed**;
- Hard gamma radiation => need to **return** the particle **back to the radiation point**, which is **not allowed in Geant4** in a simple way.

Old channeling model in Geant4

Currently implemented*
Channeling physics:

- Only trajectories (**no radiation**)
- Only for hadrons
- Changing cross-sections using **Geant4 Biasing**

To do:

- To resolve the **problems** with modification of **continuous discrete processes**
- To add channeling of **e+/e-**
- To add channeling **radiation**
- To add coherent **pair production**

Problem with modification of the **electromagnetic physics list**:
class G4ChannelingOptrChangeCrossSection

```
        switch (type) {
            case fNotDefined:
                fProcessToDensity[processName] = fDensityRatioNone;
                break;
            case fTransportation:
                fProcessToDensity[processName] = fDensityRatioNone;
                break;
            case fElectromagnetic:
                if(subType == fCoulombScattering ||
                   subType == fMultipleScattering){
                    fProcessToDensity[processName] = fCancelProcess;
                }
                if(subType == fIonisation ||
                   subType == fBremsstrahlung){
                    fProcessToDensity[processName] = fCancelProcess;
                }
                if(subType == fPairProdByCharged ||
                   subType == fAnnihilation ||
                   subType == fAnnihilationToMuMu ||
                   subType == fAnnihilationToHadrons){
```

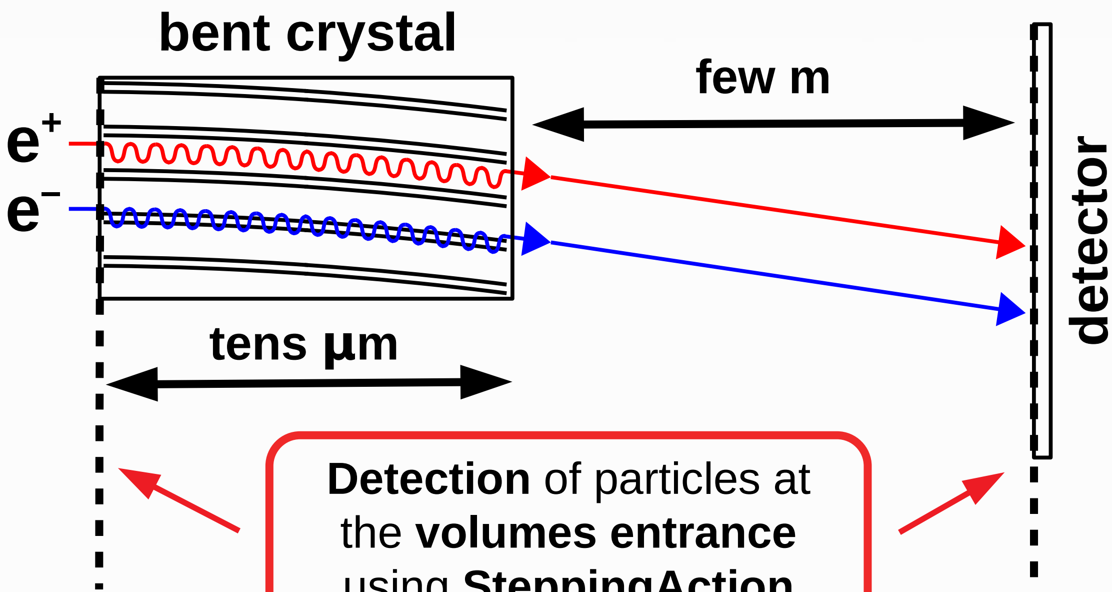
It is not possible to turn off/to modify **continuous discrete processes** (multiple scattering, ionization losses) in this way but only **discrete processes**

Crucial for e+/e-
though not so important for high energy protons

*E. Bagli Eur. Phys. J. C 74, 2996 (2014)

First Geant4 channeling example for electrons/positrons

- **Inspired by** our experiments* of **855 MeV electron** beam deflection by an ultrashort **bent crystal** at **Mainz Mikrotron MAMI**



Detection of particles at the **volumes entrance** using **SteppingAction**

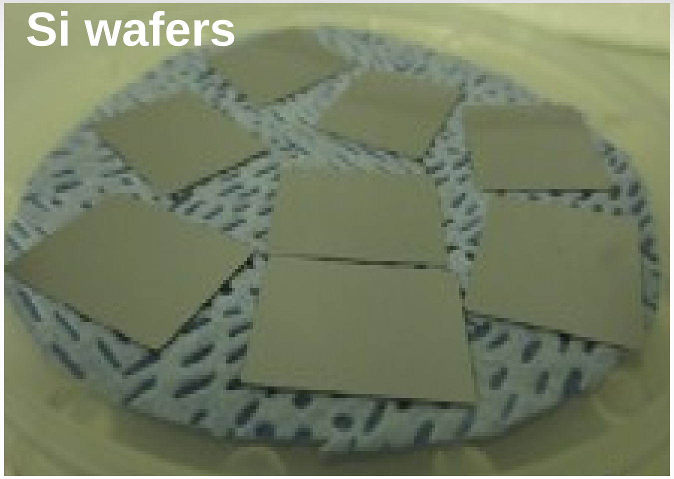
Multithreading works!
Checked at the supercomputer
Galileo100@CINECA (Italy)
NURION@KISTI (Korea)

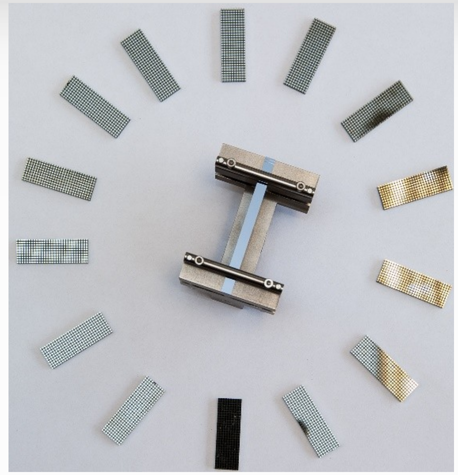
Output both in **root** (only primary particles) and in **textfile** (all the particles) format

***A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)**

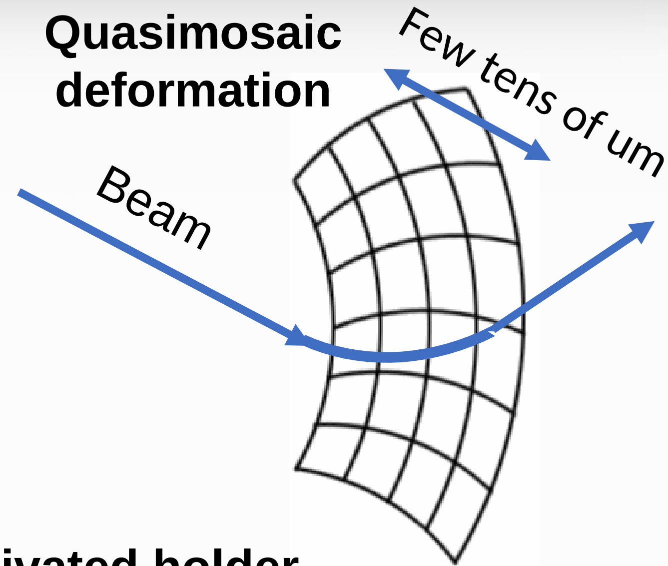
A. Sytov et al. Eur. Phys. J. C 77, 901 (2017)

Manufacturing and characterization of bent silicon crystals @INFN Ferrara

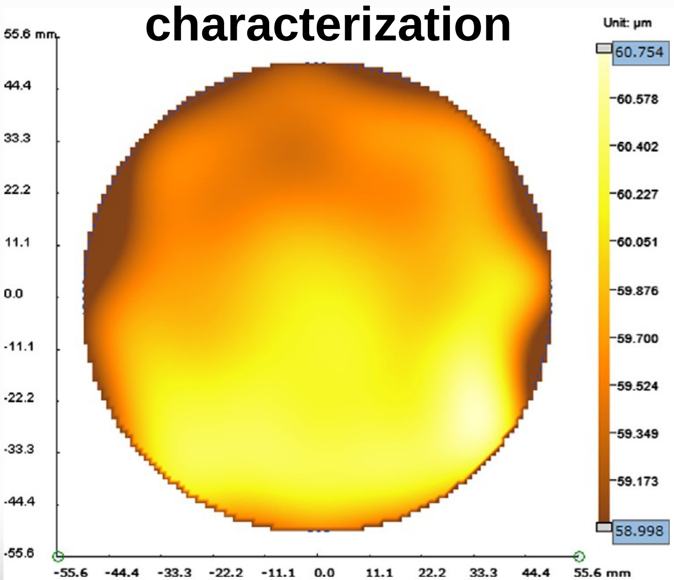




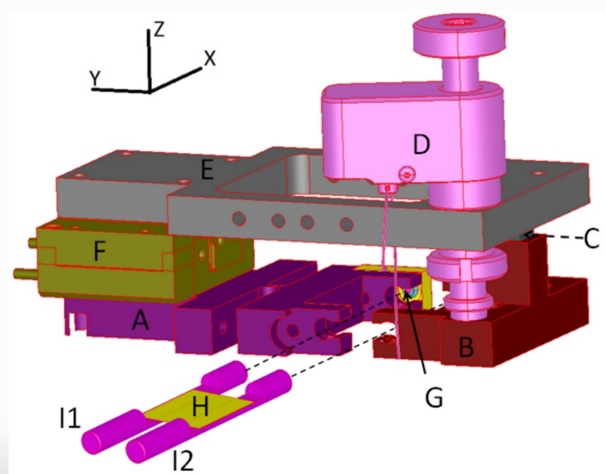
Quasimosaic deformation

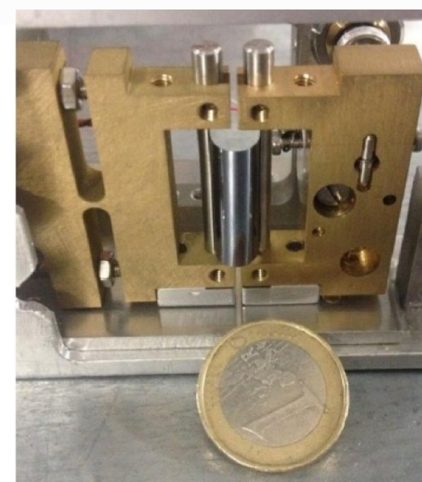


characterization



Piezo-activated holder





How to use the Geant4 channeling model in your example?

- **Add to DetectorConstruction::Construct()**

```
//crystal volume
G4Box* crystalSolid = new G4Box("Crystal",CrystalSizeX/2,CrystalSizeY/2,CrystalSizeZ/2.);
crystalLogic = new G4LogicalVolume(crystalSolid,crystalMaterial,"Crystal");
          new G4PVPlacement(xRot,posCrystal,crystalLogic,"Crystal",logicWorld,false,0);
//crystal region (necessary for the FastSim model)
fRegion = new G4Region("Crystal");
fRegion->AddRootLogicalVolume(crystalLogic);
```

Volume declaration (completely standard)

G4Region declaration

- **Add to DetectorConstruction::ConstructSDandField()**

```
void DetectorConstruction::ConstructSDandField()
{
    // -------------- fast simulation ---------------------------
    //extract the region of the crystal from the store
    G4RegionStore* regionStore = G4RegionStore::GetInstance();
    G4Region* RegionCh = regionStore->GetRegion("Crystal");

    //create the channeling model for this region
    G4ChannelingFastSimModel* ChannelingModel =
        new G4ChannelingFastSimModel("ChannelingModel", RegionCh);
    //activate the channeling model
    ChannelingModel->Input(crystalMaterial, Lattice);
    //setting bending angle of the crystal planes (default is 0)
    ChannelingModel->GetCrystalData()->
            SetBendingAngle(BendingAngle,crystalLogic);

    //activate radiation model
    if (ActivateRadiationModel) ChannelingModel->RadiationModelActivate();
}
```

Get crystal region

Channeling FastSim model declaration

Model activation and input

Optional

Radiation model activation

Update of multiple scattering theory for the crystal case (in analogy to the Bremsstrahlung theory)*

- **Coulomb scattering cross-section** on an target consisting of N atoms in general case:

$$\frac{d\sigma}{d\Omega} = \left|\sum_{j=1}^{N} e^{i\mathbf{q}\mathbf{r_j}}\right|^2 \frac{d\sigma_{at}}{d\Omega} \quad (1)$$

- **Coulomb scattering cross-section** on an amorphous target consisting of N atoms:

$$\frac{d\sigma_{am}}{d\Omega} = N\frac{d\sigma_{at}}{d\Omega} \quad (2)$$

- For the **crystal case** the cross-section is divided onto the **coherent** and **incoherent** ones**:**

$$\frac{d\sigma_{cr}}{d\Omega} = \frac{d\sigma_{coh}}{d\Omega} + \frac{d\sigma_{inc}}{d\Omega} \quad (3)$$

where **coherent scattering cross-section:**

$$\frac{d\sigma_{coh}}{d\Omega} = D\left|\sum_{j=1}^{N} e^{i\mathbf{q}\mathbf{r_{j0}}}\right|^2 \frac{d\sigma_{at}}{d\Omega}$$

incoherent scattering cross-section:

$$\frac{d\sigma_{inc}}{d\Omega} = N(1-D)\frac{d\sigma_{at}}{d\Omega} = \frac{d\sigma_{am}}{d\Omega} - \frac{d\sigma_1}{d\Omega}$$

Debye-Waller factor (D)

*Submitted to Eur. Phys. J. C

Update of multiple scattering theory for the crystal case: Coherent scattering suppression effect*

- The **cross-section** for a **crystal** may be either **higher** or **lower** than for amorphous target:

$$\frac{d\sigma_{cr}}{d\Omega} = \frac{d\sigma_{coh}}{d\Omega} + \frac{d\sigma_{inc}}{d\Omega} \qquad (1)$$

Depends on the crystal alignment

- **At certain crystal alignment coherent scattering ➔ 0:**

$$d\sigma \xrightarrow{d\sigma_{coh}=0} d\sigma_{am} - d\sigma_1$$

we call this effect ***Coherent scattering suppression*** (***CSS***)

- The **minimal scattering angle** in the **G. Molière** theory** ϑ_{min}^{am} transforms for the **crystal** case into:

$$\ln \vartheta_{min}^{cr} = \ln \vartheta_{min}^{am} + \frac{0.5Z}{Z+1}\left[\left(1+\frac{u_1^2}{R^2}\right) e^{\frac{u_1^2}{R^2}} E_1\left(\frac{u_1^2}{R^2}\right) - 1\right]$$

➔ **Molière angular distribution**

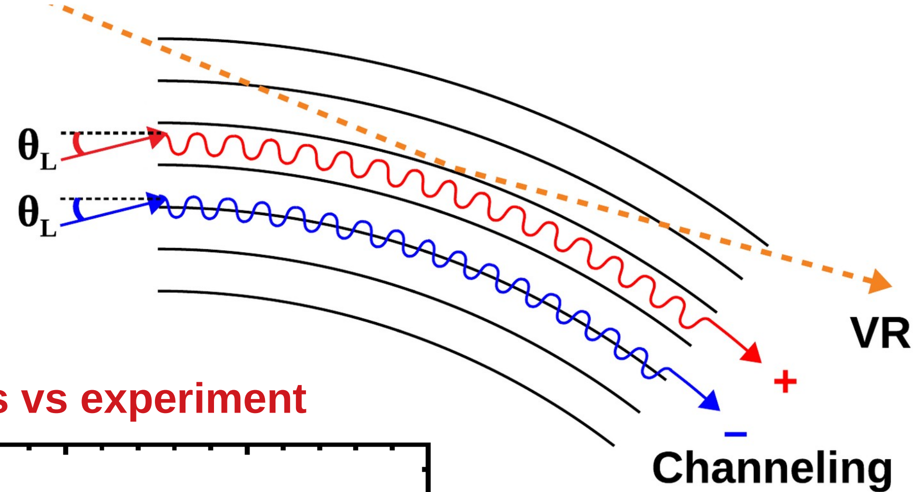
****G. Molière, Z. Naturforschg. 3A, 78-97 (1948); H.A. Bethe Phys. Rev. 89, 6 (1953)**

***Submitted to Eur. Phys. J. C**

Geant4 channeling model validation: beam deflection by a bent crystal

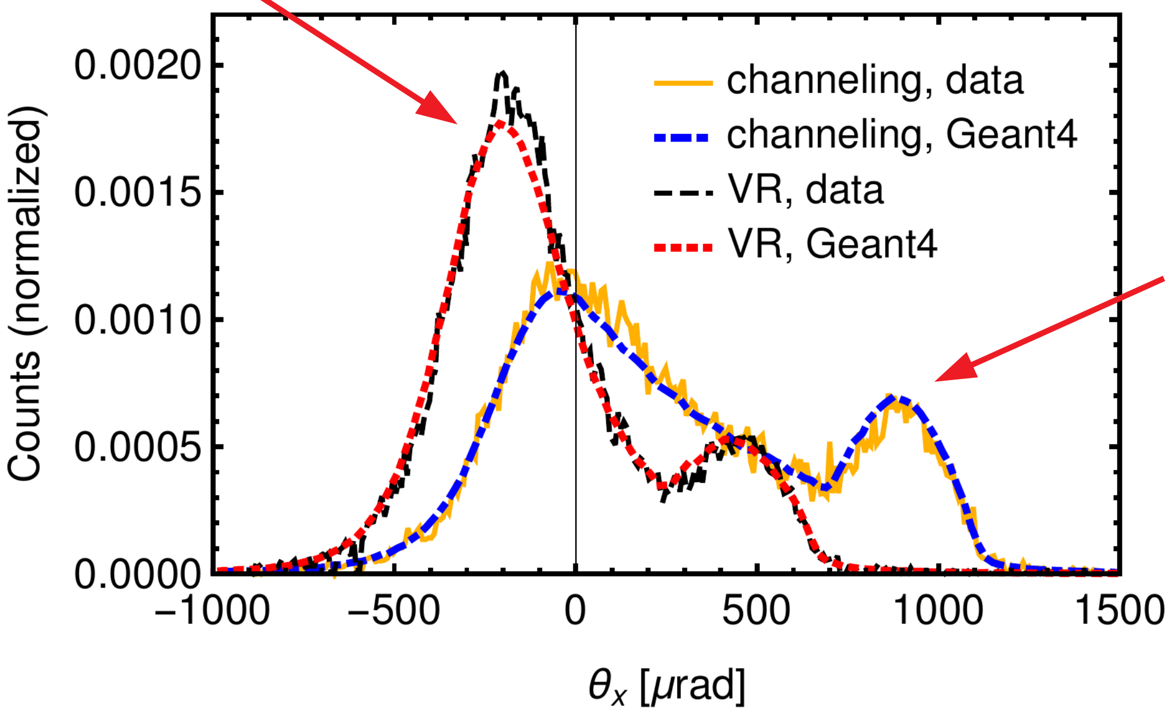
855 MeV electrons

15 µm thick bent crystal



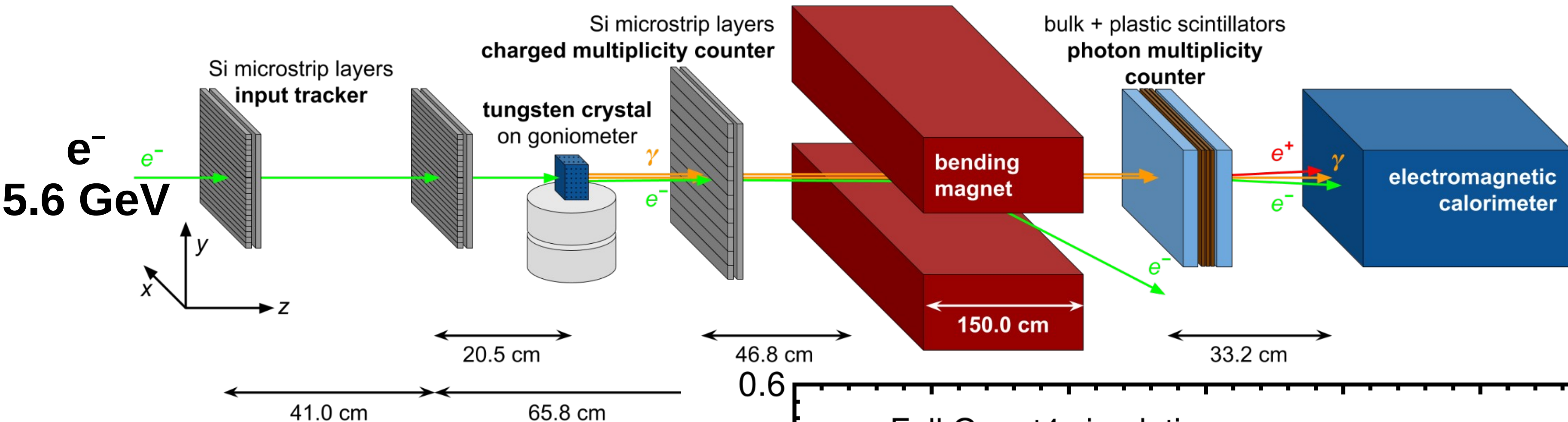
volume reflection (VR)

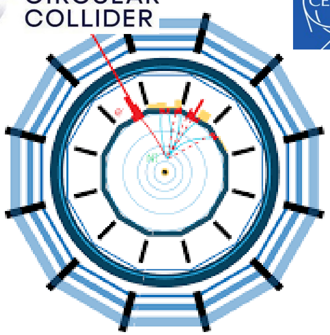
Geant simulations vs experiment

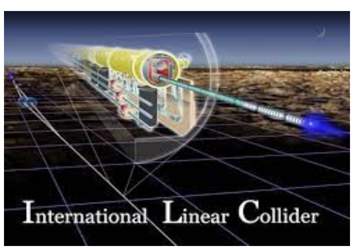


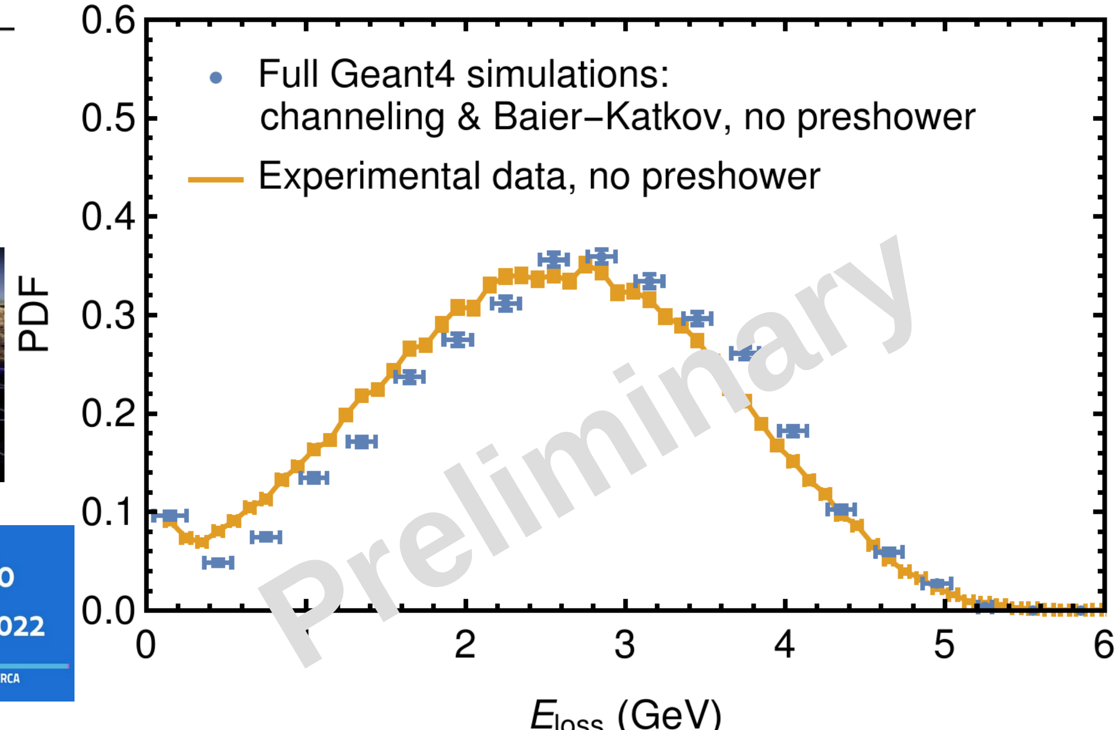
channeling

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



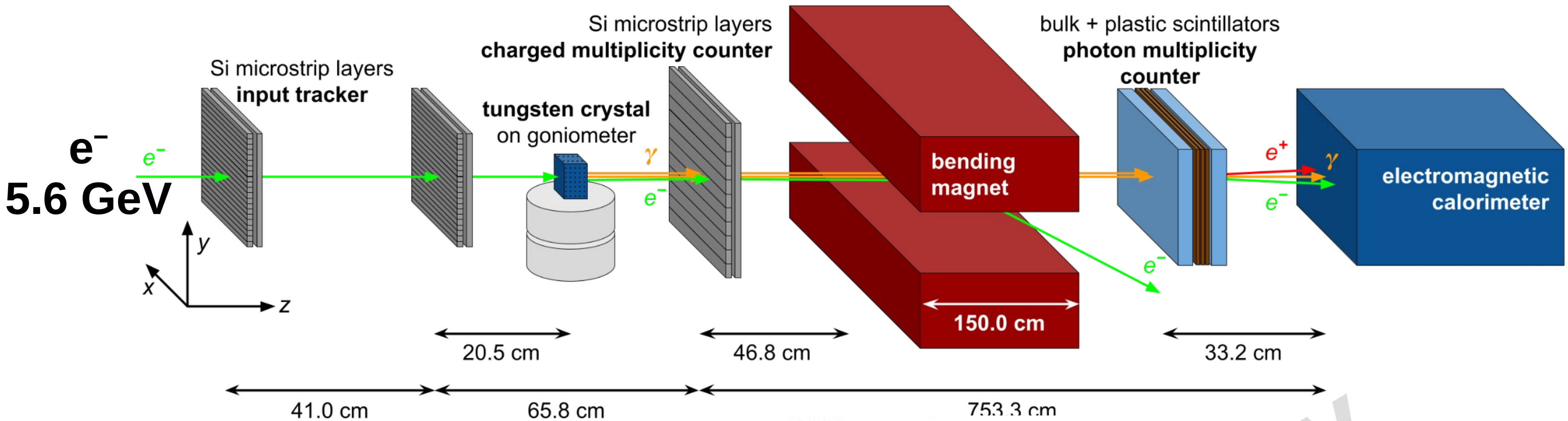




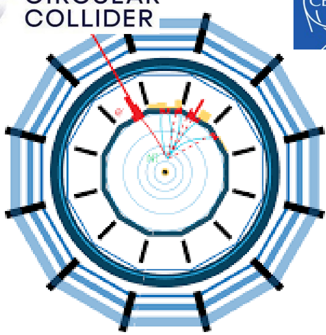


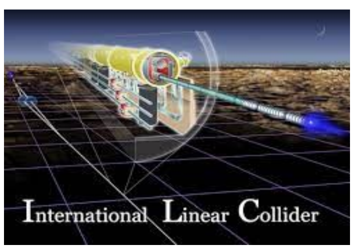
Intense positron source Based On Oriented crySTals - e+BOOST
(PI L. Bandiera)
PRIN2022-2022Y87K7X
Financed by Italian Ministry of University and Research - PRIN project

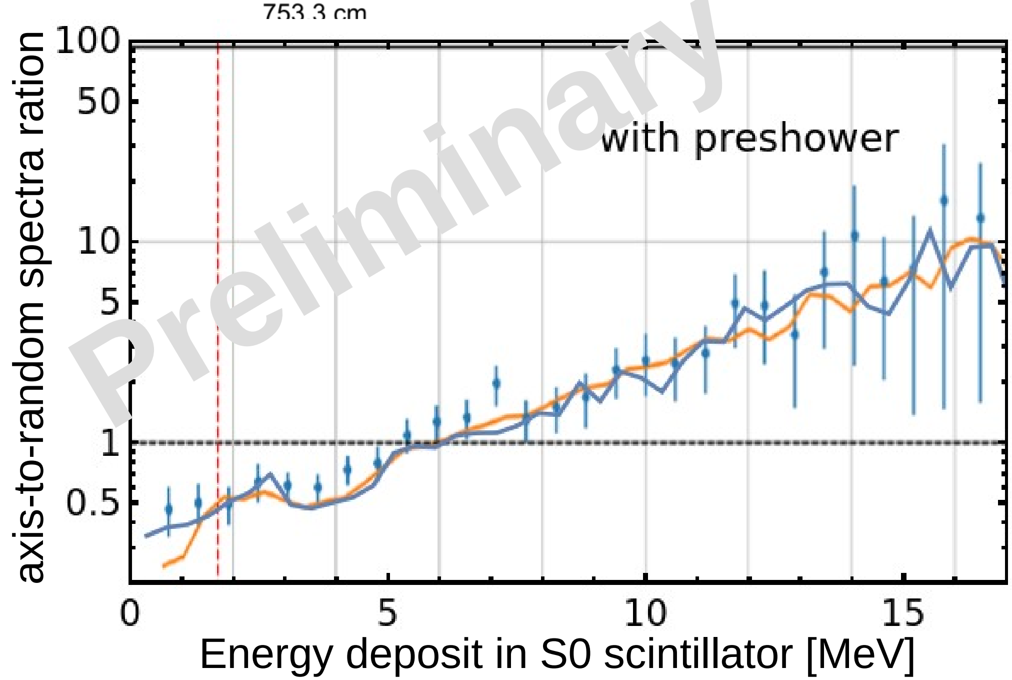
Full Geant4 simulations of the DESY experiment* for the FCC-ee positron source project



FUTURE CIRCULAR COLLIDER







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