Geant4 channeling and Baier-Katkov models and their applications in accelerator physics, particle physics and space science

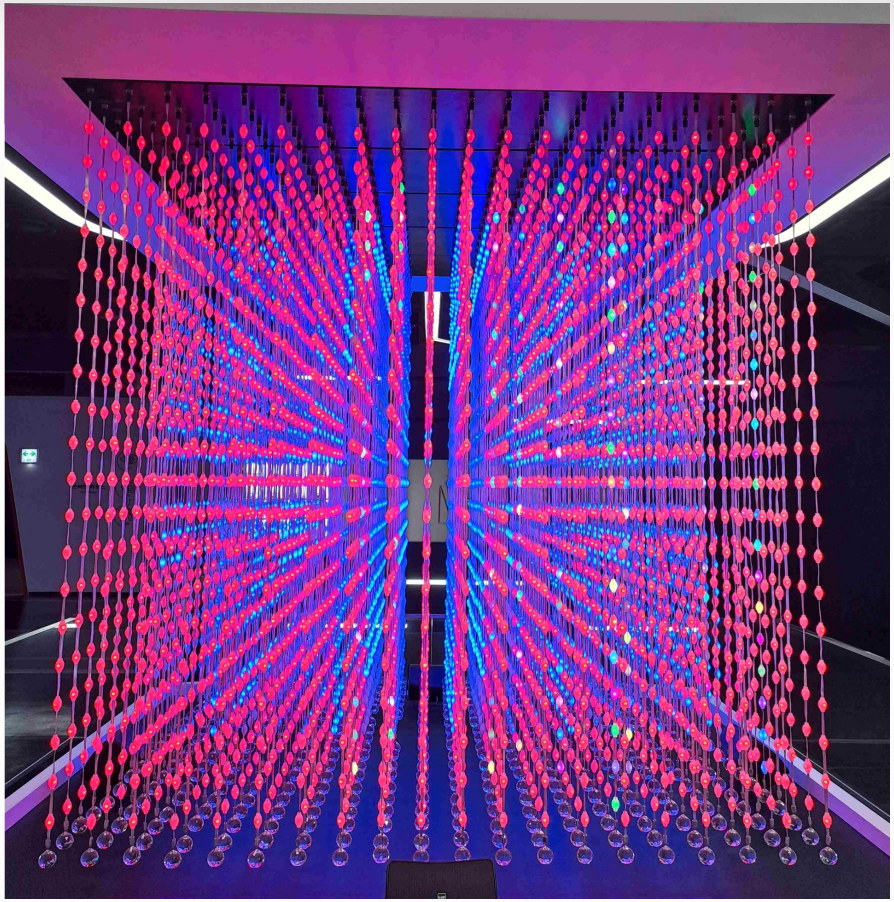
A. Sytov, L. Bandiera, K. Cho, G.A.P. Cirrone, S. Guatelli, V. Haurylavets, S. Hwang, V. Ivanchenko, L. Pandola, G. Paternò, A. Rosenfeld, V. Tikhomirov

sytov@fe.infn.it

28th Geant4 Collaboration Meeting

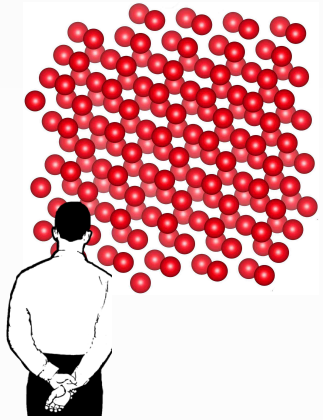
Sapporo, 2023/09/25

How an oriented crystal looks like

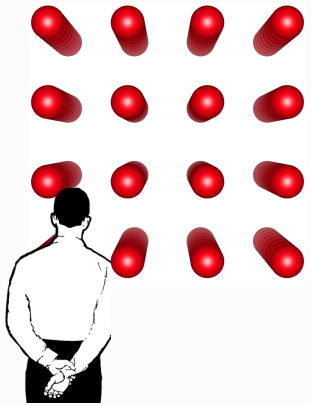


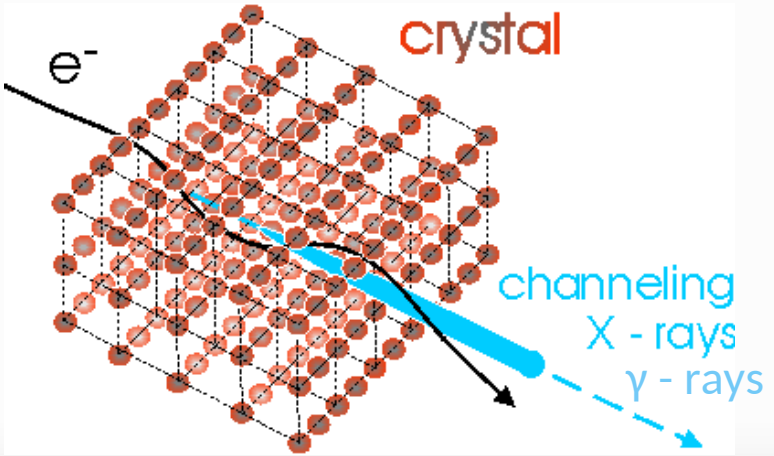
from National Science Museum, Daejeon, Korea

Non-oriented crystal



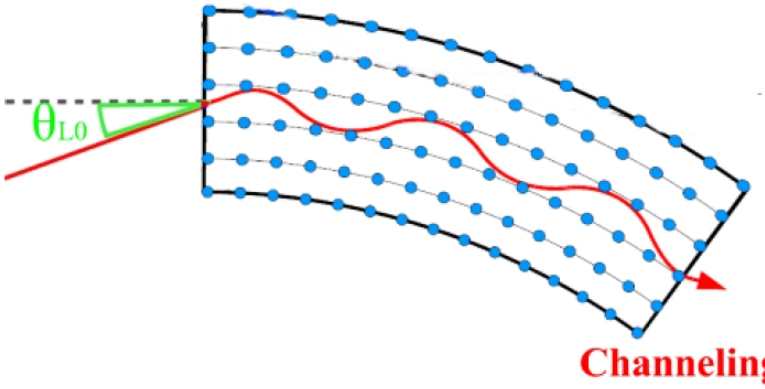
Oriented crystal



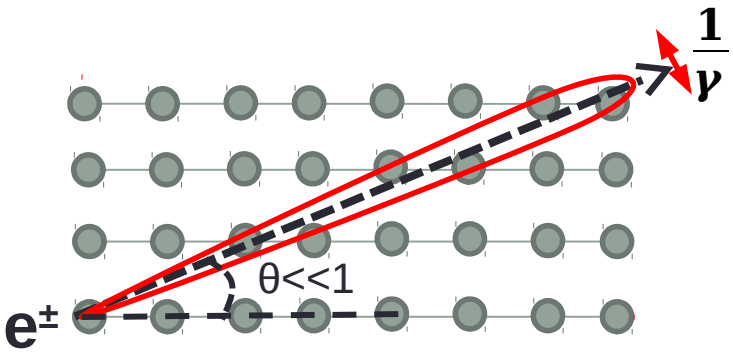


The idea: MC simulations of coherent effects in a crystal

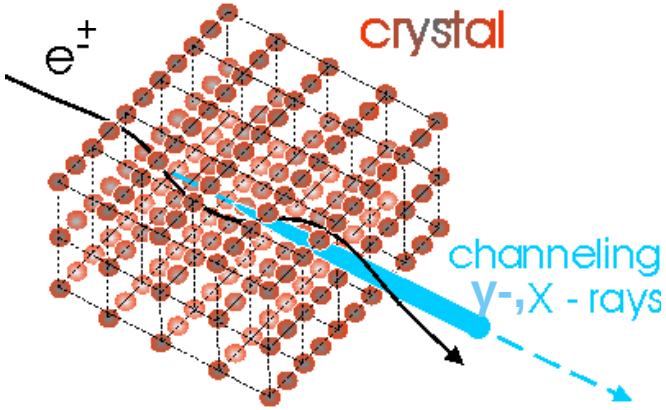
Channeling*



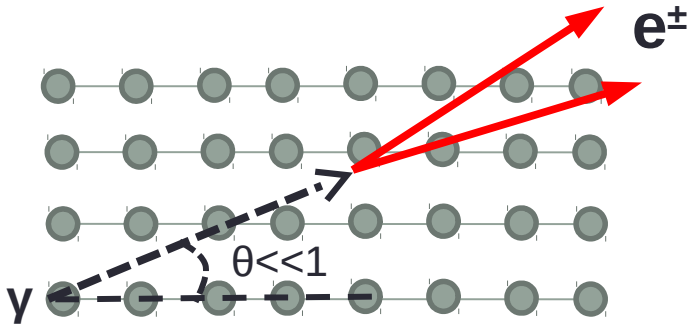
Coherent bremsstrahlung***



Channeling radiation**



Coherent pair production****



*J. Stark, Zs. Phys. 13, 973–977 (1912); J. A. Davies, J. Friesen, J. D. McIntyre, Can J. Chem. 38, 1526–1534 (1960)

**M.A. Kumakhov, Phys. Lett. A 57(1), 17–18 (1976)

***B. Ferretti, Nuovo Cimento 7, 118 (1950); M. Ter-Mikaelian, Sov. Phys. JETP 25, 296 (1953).

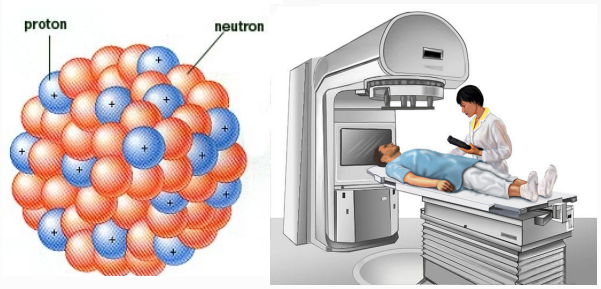
**** H. Überall, Phys. Rev. 103, 1055 (1956).

Applications of oriented crystals*

European Commission

Trillion

X and y-ray source for nuclear physics and cancer radiotherapy

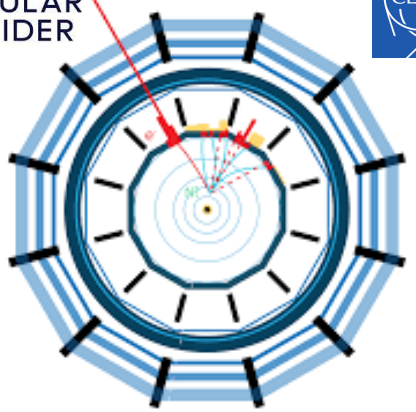


Gamma-ray Space Telescope

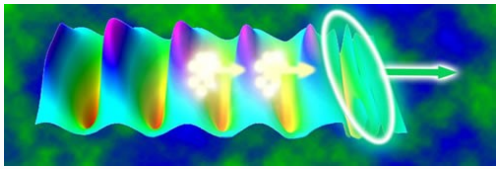
Positron source for future multi-billion € e+/e- and muon colliders

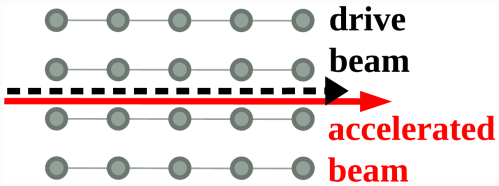
FUTURE CIRCULAR COLLIDER

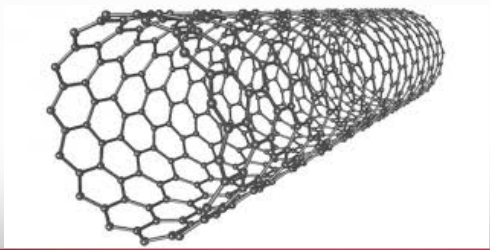
CERN



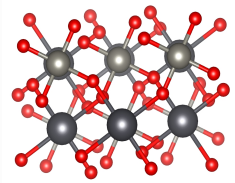
Plasma wakefield acceleration







Oriented crystals



Crystal-based beam extraction from accelerators and colliders

*A. Sytov et al., JKPS, https://doi.org/10.1007/s40042-023-00834-6

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:

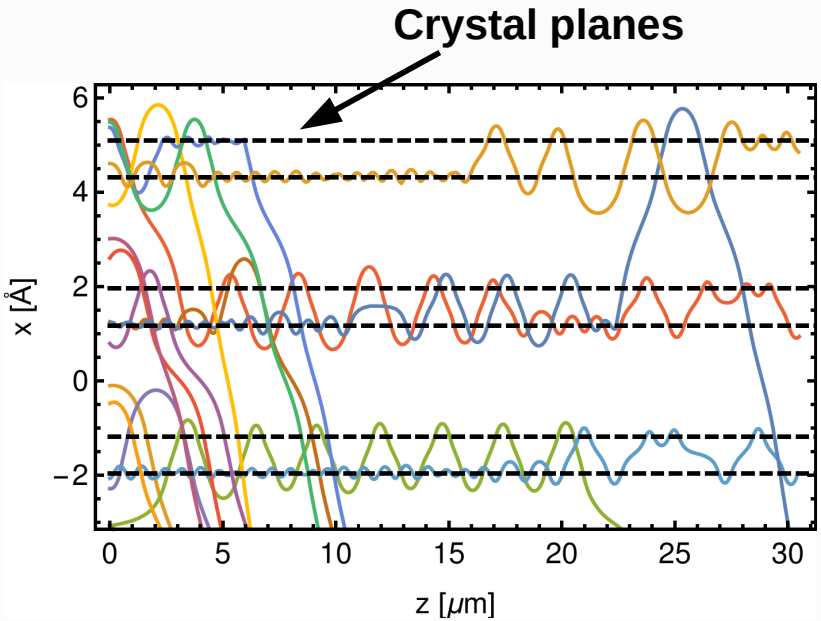
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

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)

Baseline channeling simulation technique: CRYSTALRAD Monte Carlo simulation code

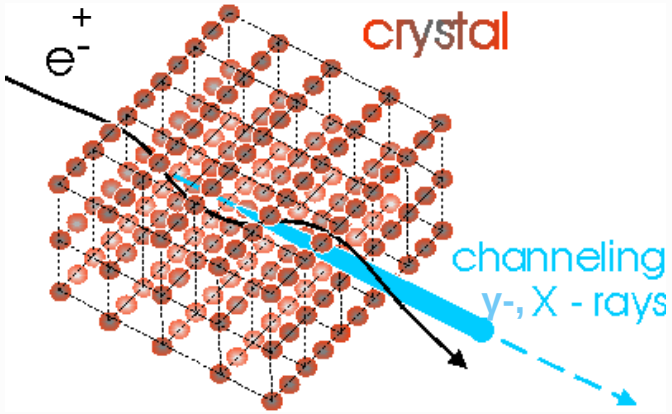
Main conception – simulation of classical trajectories of charged particles in a crystal in averaged atomic potential of planes or axes. Multiple and single **scattering simulation** at every step



channeling*

Advantages:

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



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. Sytov et al. JKPS 83, 132–139 (2023)

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.

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

```
71  G4bool TestModel::IsApplicable(const G4ParticleDefinition& particleType)
72  {
73    return
74      &particleType == G4Proton::ProtonDefinition()||
75      &particleType == G4AntiProton::AntiProtonDefinition()||
76      &particleType == G4Electron::ElectronDefinition() ||
77      &particleType == G4Positron::PositronDefinition();// ||
78      //&particleType == G4Gamma::GammaDefinition();
79  }
80
81  //....oooOOOOOooo........oooOOOOOooo........oooOOOOOooo........oooOOOOOooo......
82
83  G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
84  {
102 }
103
104 //....oooOOOOOooo........oooOOOOOooo........oooOOOOOooo........oooOOOOOooo......
105
106 void TestModel::DoIt(const G4FastTrack& fastTrack,
107                      G4FastStep& fastStep)
108 {
```

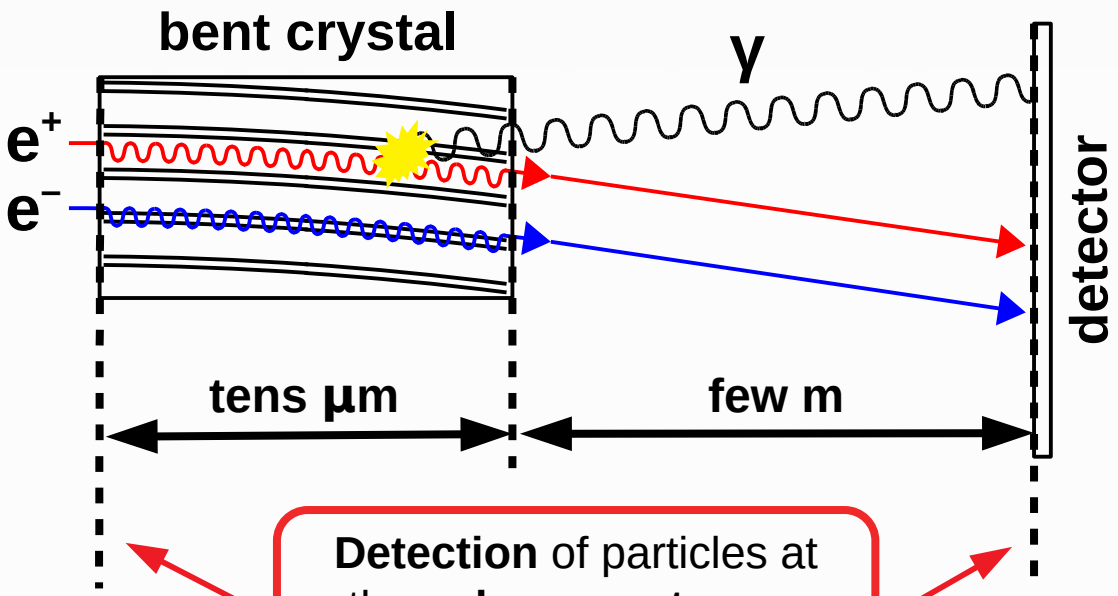
Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

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**

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

Beam setup in **run.mac** using **GPS** commands; all the **geometry** in **DetectorConstruction**

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

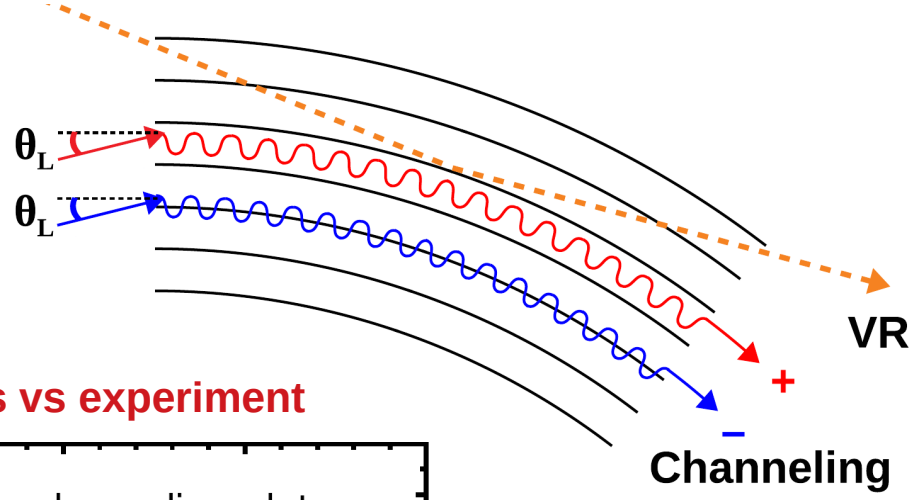
*A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

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

First simulations with Geant4 channeling model: beam deflection by a bent crystal

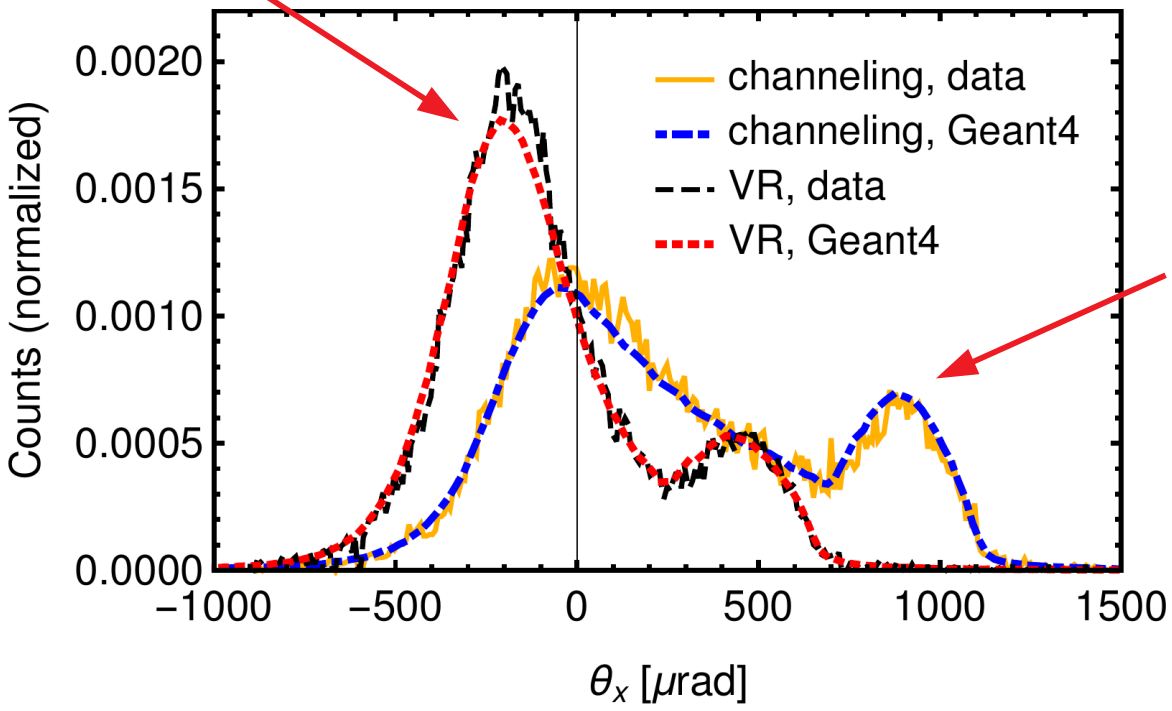
855 MeV electrons

15 μm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



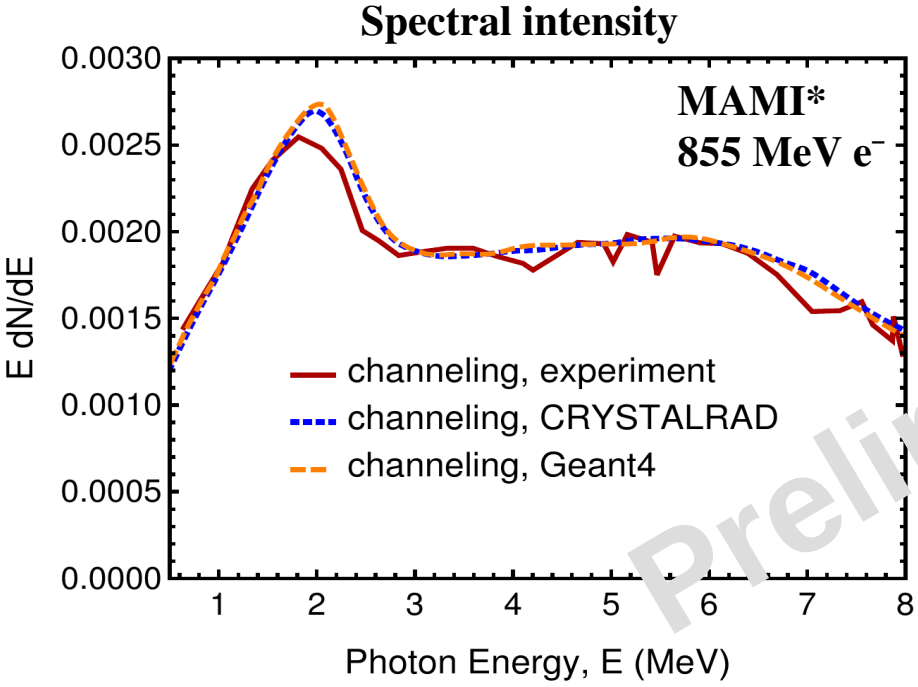
channeling

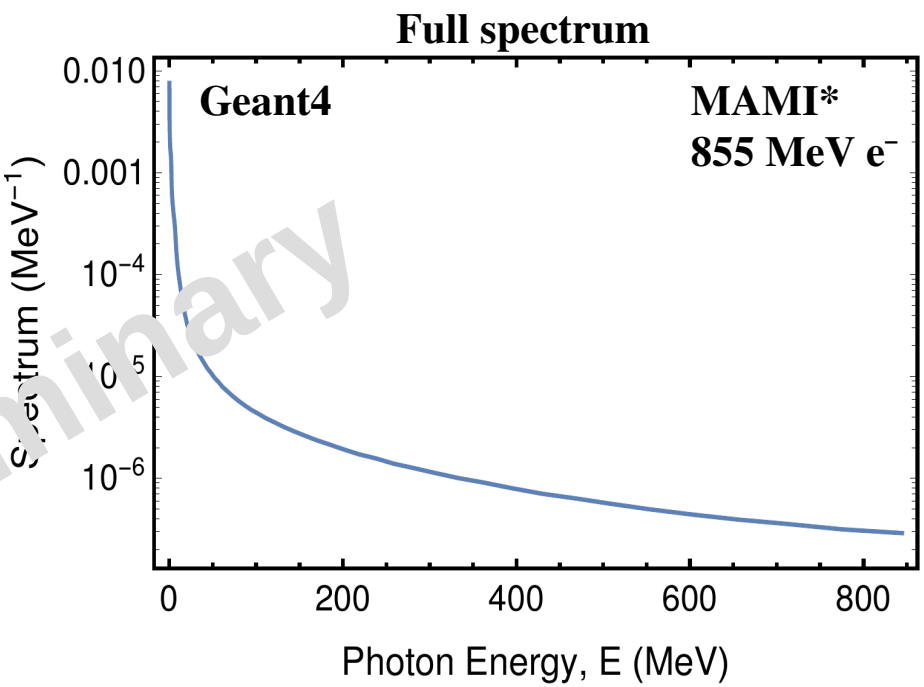
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

G4BaierKatkov:

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

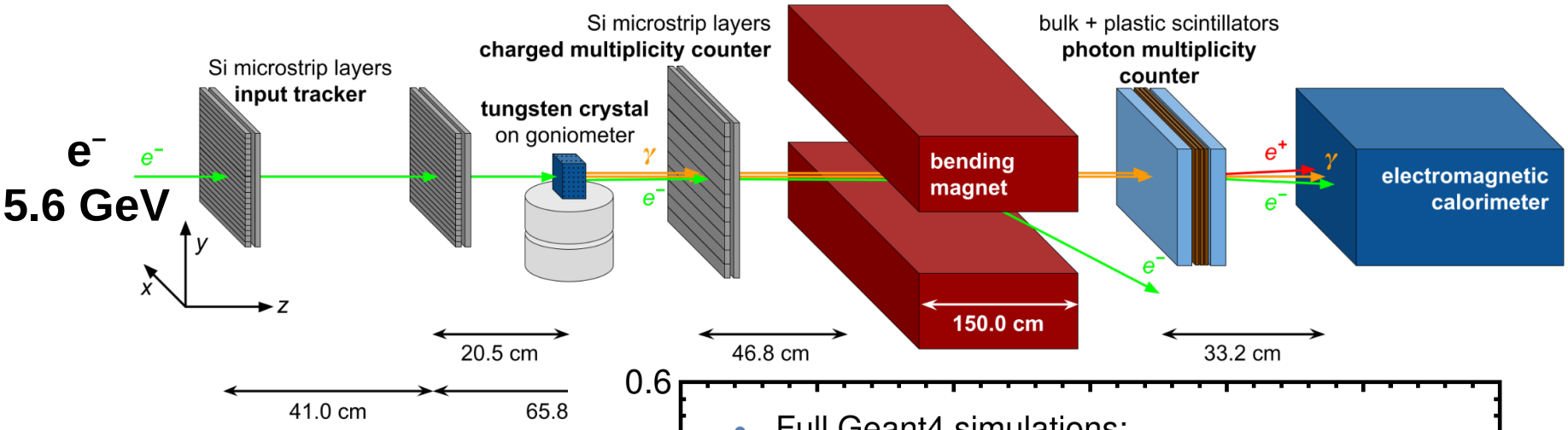
Geant simulations vs experiment and CRYSTALRAD simulations

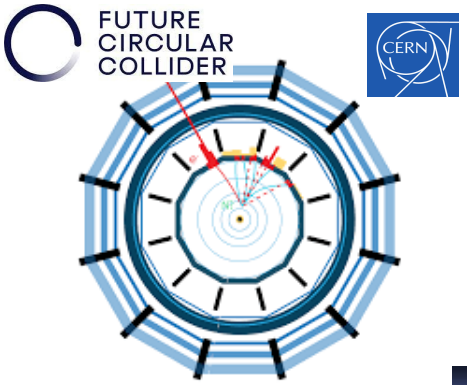


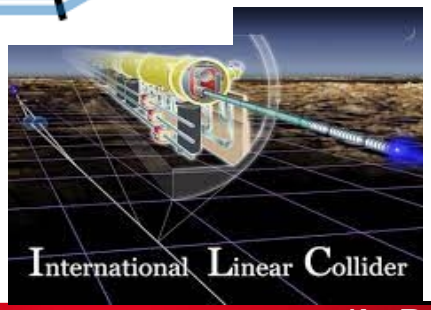


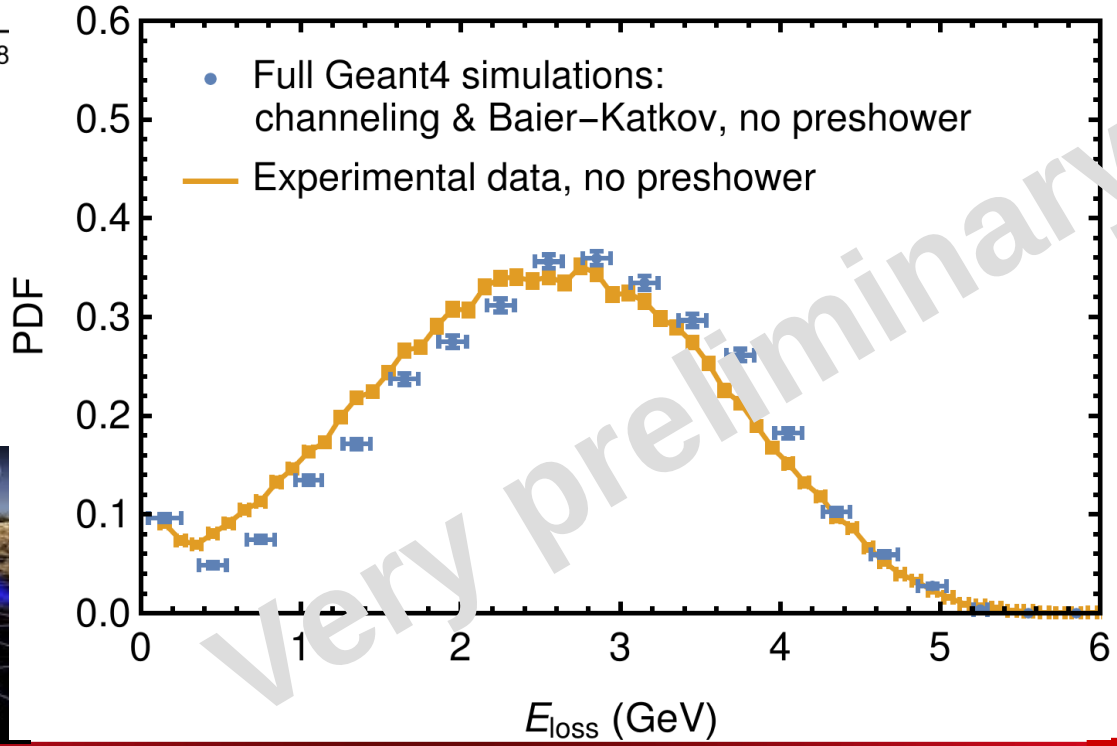
*L. Bandiera et al. Phys. Rev. Lett. 115, 025504 (2015)

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









*L. Bandiera et al. Eur. Phys. J. C 82, 699 (2022)

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

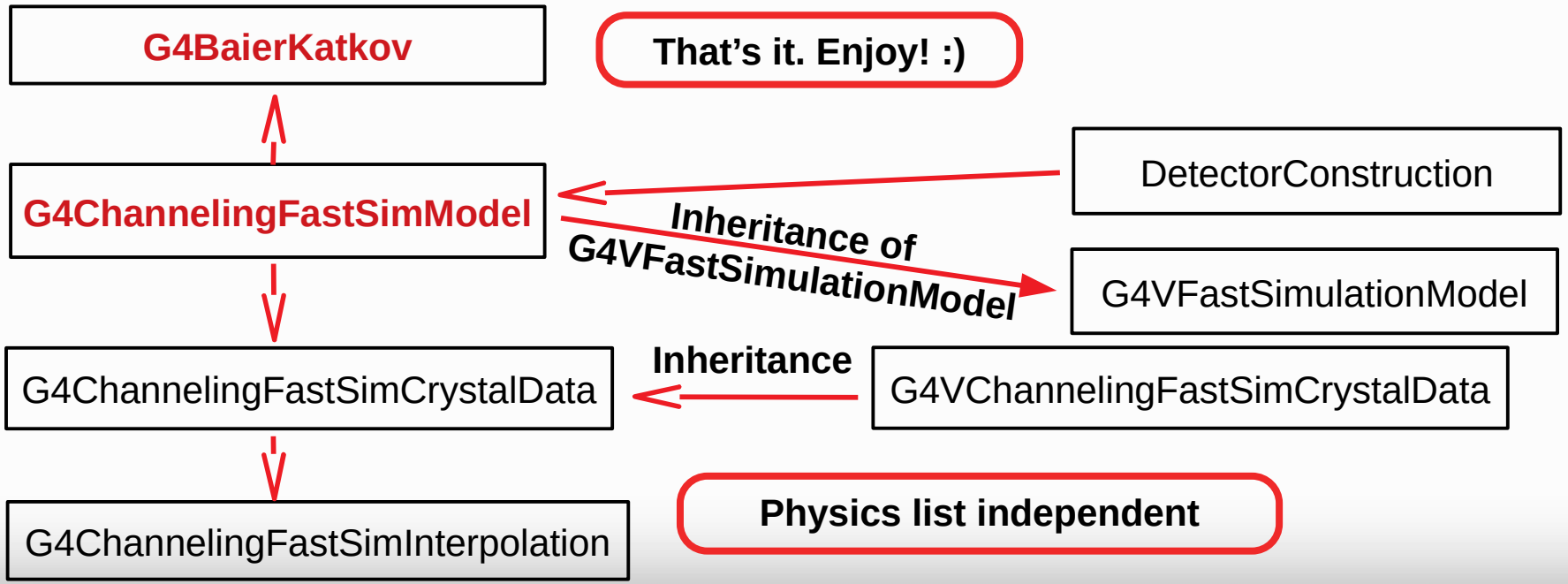
Radiation model activation

How to use the Geant4 channeling model in your example?

- **Add to main:**

Register FastSimulationPhysics

```
G4FastSimulationPhysics* fastSimulationPhysics = new G4FastSimulationPhysics();
fastSimulationPhysics->BeVerbose();
// -- activation of fast simulation for particles having fast simulation models
// -- attached in the mass geometry:
fastSimulationPhysics->ActivateFastSimulation("e-");
fastSimulationPhysics->ActivateFastSimulation("e+");
// -- Attach the fast simulation physics constructor to the physics list:
physicsList->RegisterPhysics( fastSimulationPhysics );
```



Current status

Already in Geant4 kernel!

Geant4-11.2.0.beta
Please use it!

Don't hesitate to contact me in the case of any problems/issues/suggestions
sytov@fe.infn.it

Please cite our papers if you use our model:

1. A. Sytov et al. JKPS 83, 132–139 (2023)
2. A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

Conclusions

- The goal **of TRILLION** is to implement **electromagnetic processes in oriented crystals** into **Geant4** which will bring to a large scientific and industrial community most of possible applications of a crystal.

- **G4ChannelingFastSimModel** is our implementation of channeling physics and Baier-Katkov method into **Geant4**. We produced the **first results** on channeling and channeling radiation. We carried out these simulations at **NURION@KISTI** and **Galileo100@CINECA** supecomputers using **Geant4 multithreading**.

- **G4ChannelingFastSimModel and G4BaierKatkov** models were released in **Geant4-11.2.0.beta**.

- The Geant4 examples that will be developed can be **applied** in **nuclear** and **medical physics** (radiation source), at e-/e+ colliders – **ILC**, **FCC-ee** and **muon collider** (positron source) and at all **e-/e+ synchrotrons** existing in the world (crystal-based beam extraction).

- Additional applications are ultrashort crystalline **calorimeter**, exotic particles **MDM** and **EDM measurement**, and **plasma wakefield acceleration**.

Acknowledgments

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

- **MC-INFN** project (INFN Geant4 group);
- **INFN OREO** project;
- **INFN GALORE** project;
- **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!

Thank you for attention!