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New Geant4 model of channeling in crystals and its potential applications in medical physics

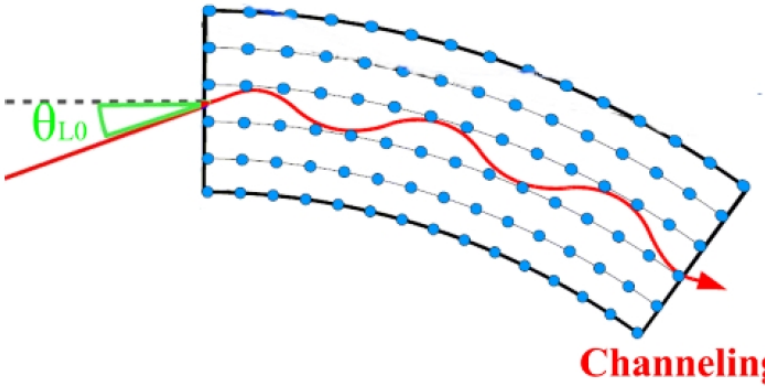
Dr. Alexei Sytov

27th Geant4 Collaboration Meeting

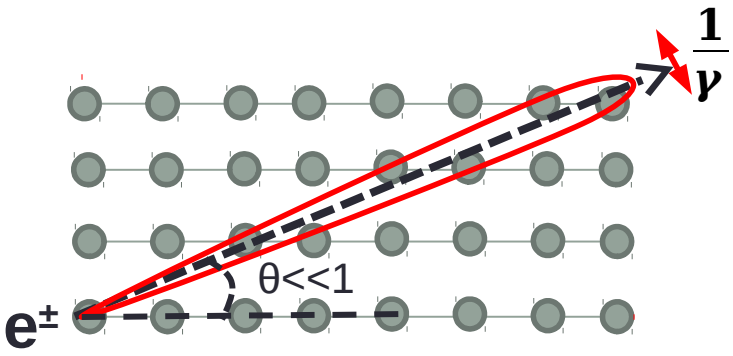
Rennes, 27/09/22

The idea: MC simulations of coherent effects in a crystal

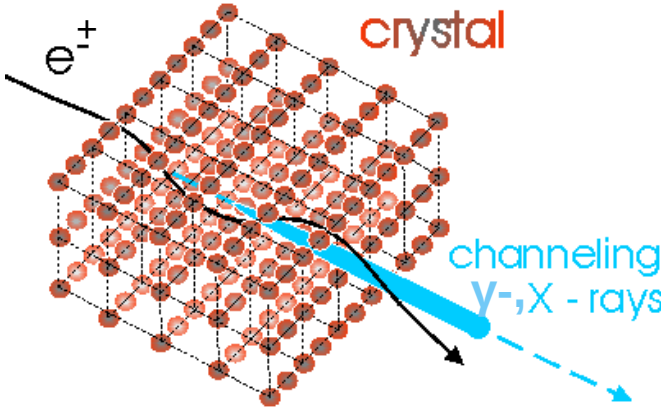
Channeling*



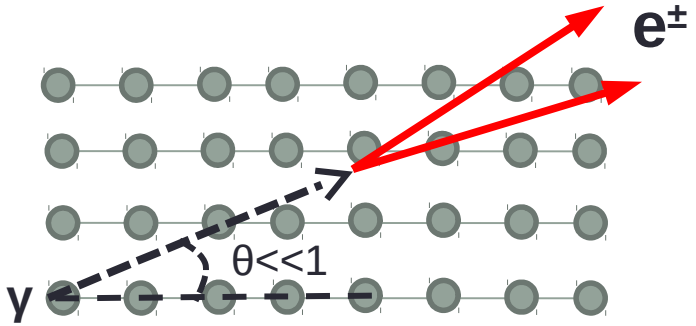
Coherent bremsstrahlung***



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).

Marie Sklodowska-Curie Action Global Individual Fellowships by A. Sytov in 2021-2024, 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:

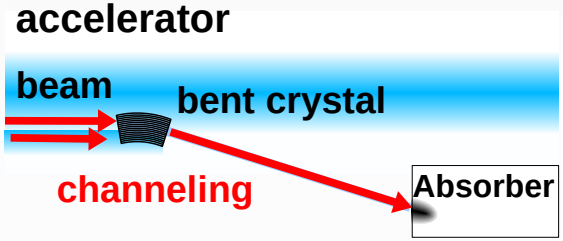
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

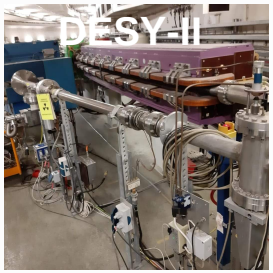
Location:

- 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)

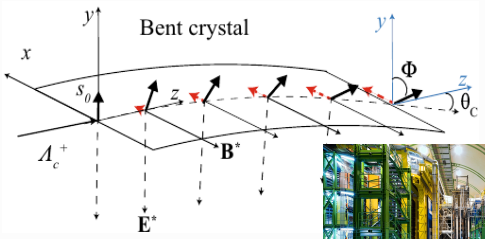
Applications*

Crystal-based collimation or beam extraction from an accelerator

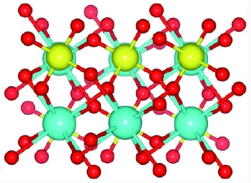




Measurement of dipole magnetic and electric moments of exotic particles

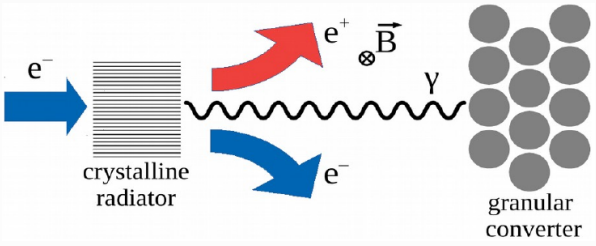


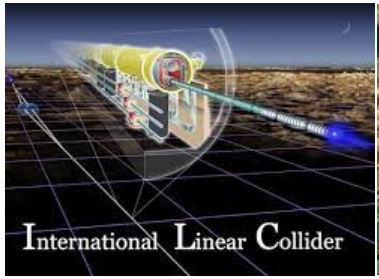
Ultrashort crystalline calorimeter



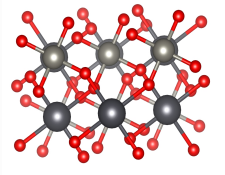
Gamma-ray Space Telescope

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

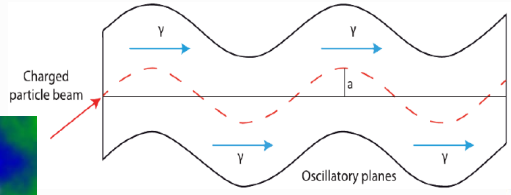


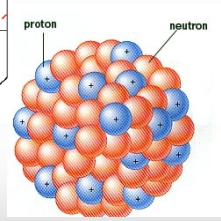


Oriented crystals

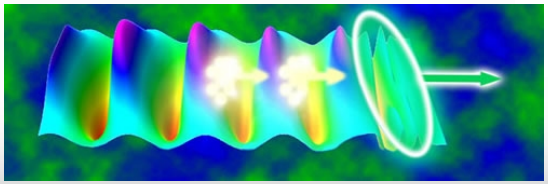


X and γ-ray source for nuclear and medical physics





Plasma acceleration



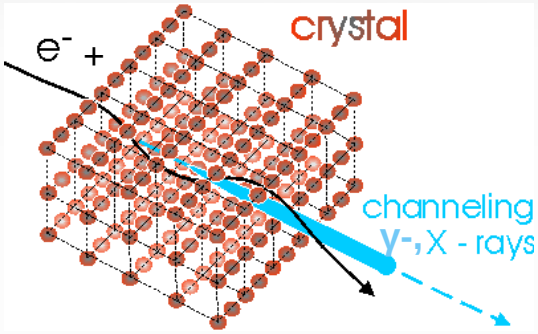
*From A. Sytov presentation at the European Researchers' Night 2021

Baseline simulation code: CRYSTALRAD

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**
- **Ionization energy losses**
- **Crystal geometry**

Baier-Katkov formula:

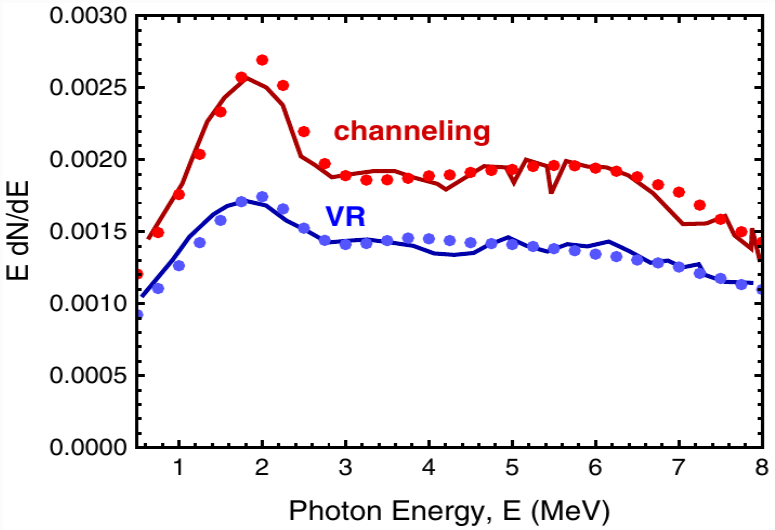
integration is made over the classical trajectory

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

Advantages:

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

CRYSTALRAD *vs* experiment



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)

Geant4 FastSim interface

A. Sytov thanks **Prof. Vladimir Ivanchenko** (**CERN**) for this solution and the group of **Prof. Pablo Cirrone** (**INFN LNS**), in particular **Dr. Luciano Pandola** as well as **Prof. Kihyeon Cho** and **Dr. Kyungho Kim** (**KISTI**), **Prof. Susanna Guatelli** and **Prof. Anatoly Rosenfeld** (**University of Wollongong**) for fruitful discussions!

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 {
```

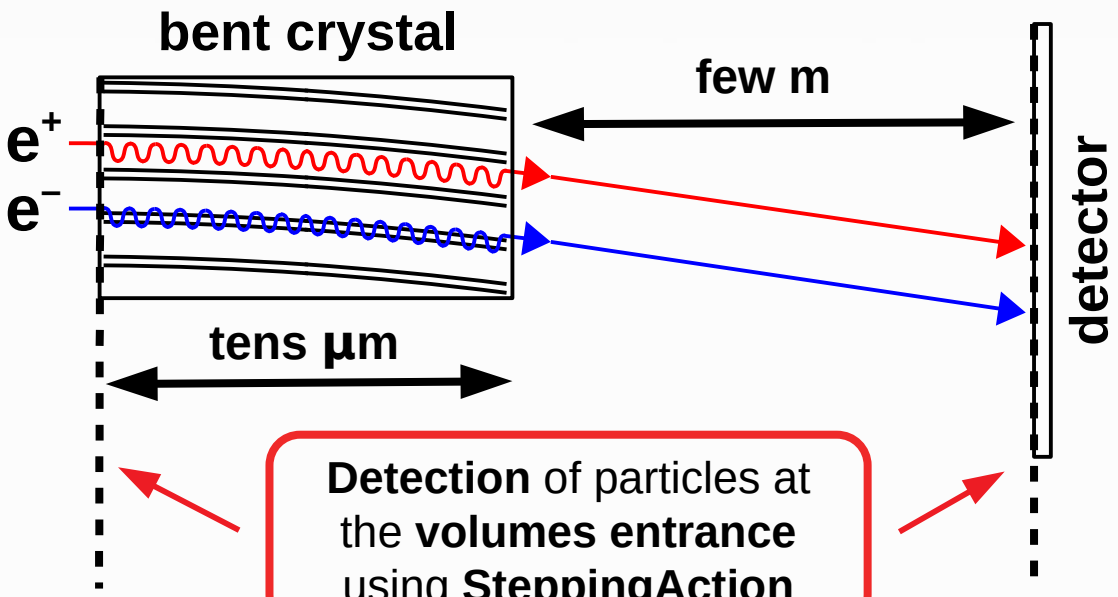
Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

First Geant4 channeling example for electrons/positrons: ChannelingFastSimModel

- **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 **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

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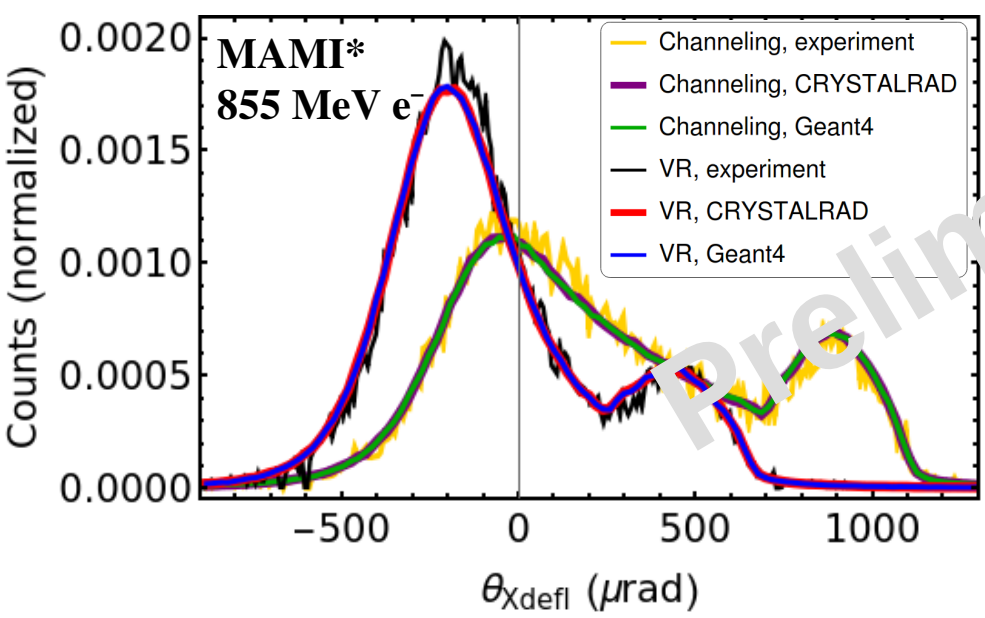
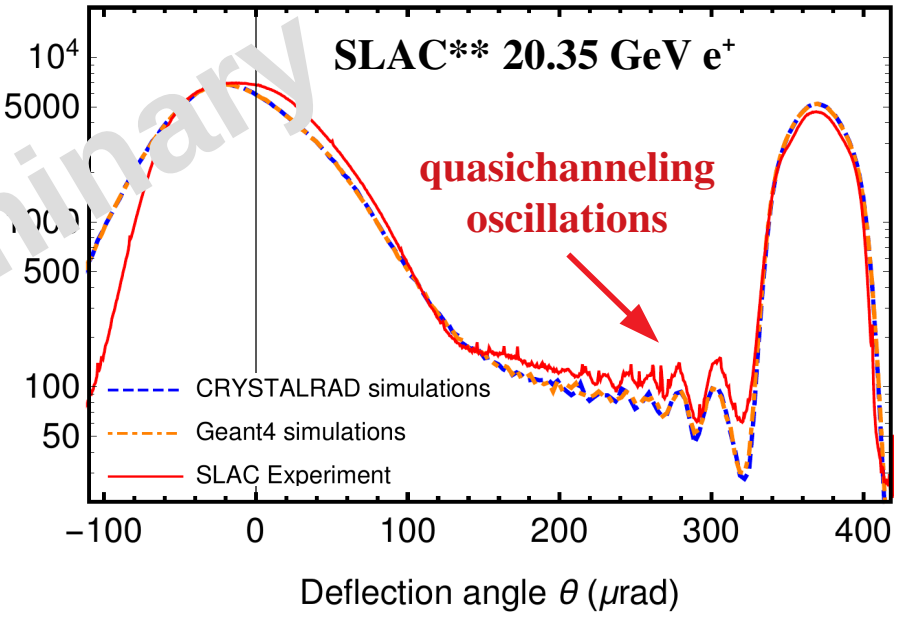
GEANT4
A SIMULATION TOOLKIT

Geant simulations vs experiment and CRYSTALRAD simulations





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

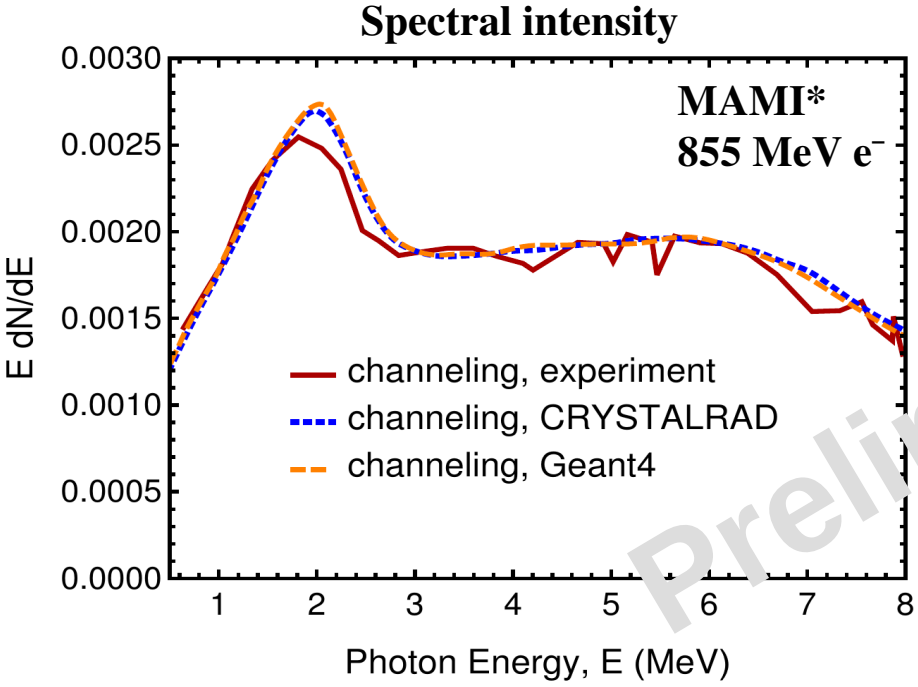
**T. N. Wistisen, …, and A. Sytov. Phys. Rev. Lett. 119, 024801 (2017)

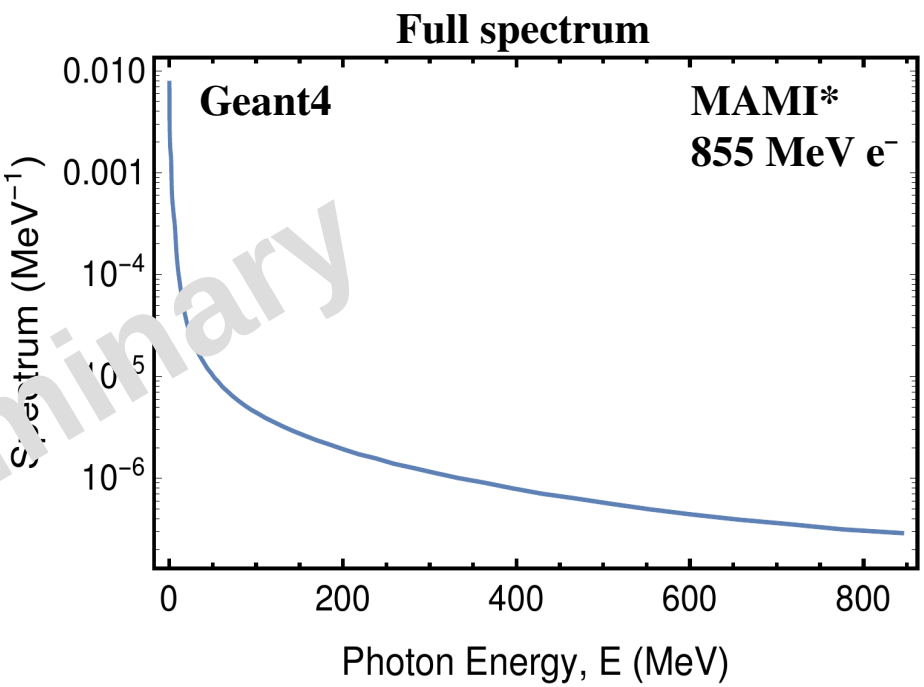
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

G4BaierKatkov:

- **Physics list independent**
- Activated in the **DetectorConstruction** and used in **ChannelingFastSimModel**
- Can be used **outside channeling model** (e.g. in **SteppingAction**)
- Provides **radiation spectrum** for single-photon radiation mode
- Provides generation of **secondary photons**

Geant simulations vs experiment and CRYSTALRAD simulations





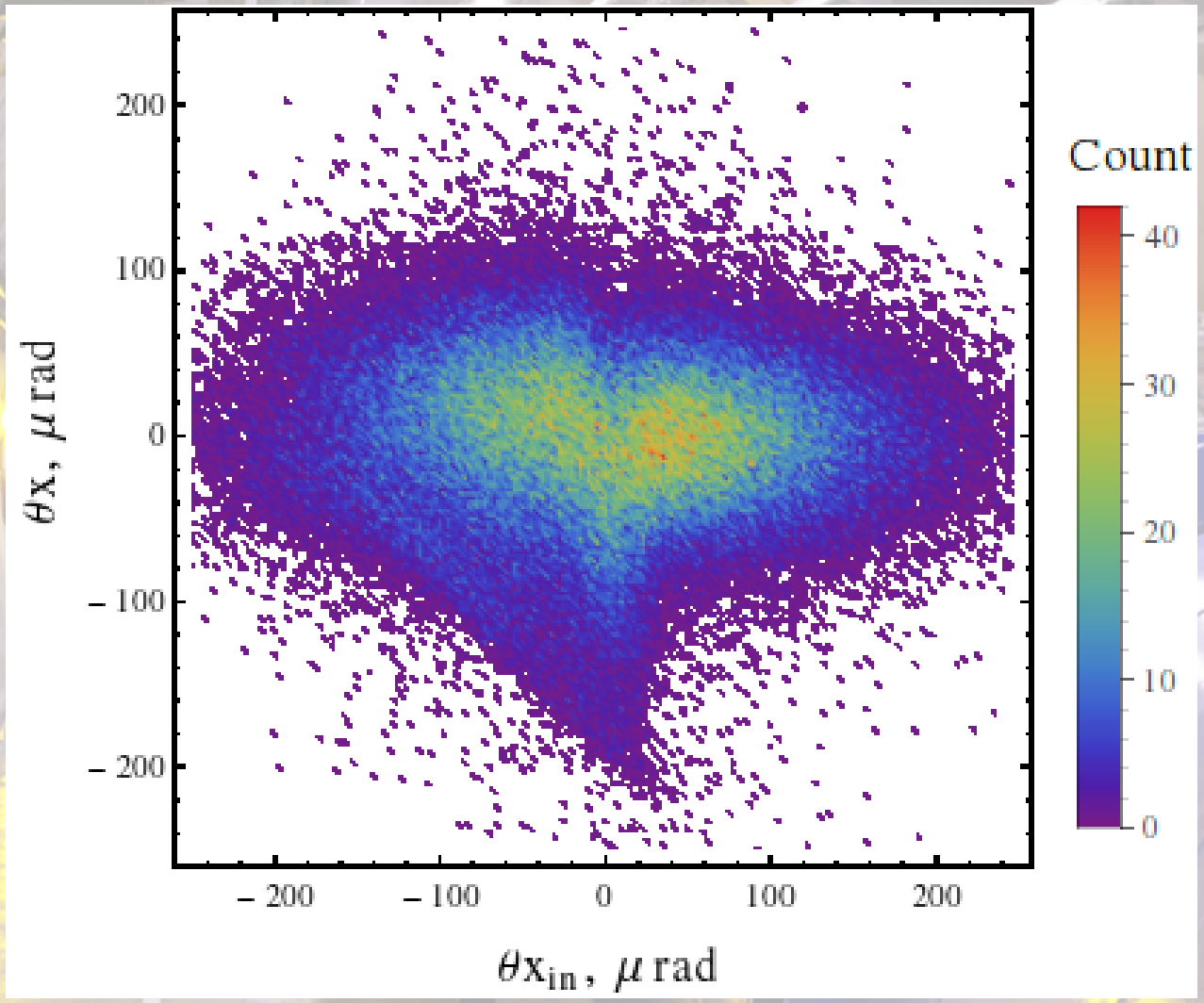
*L. Bandiera et al. Phys. Rev. Lett. 115, 025504 (2015)

New channeling model implementation into Geant4

The channeling model is ready to be inserted into the next Geant4 release

To implement:

- **Channeling** model using FastSim interface: **READY**
  (only trajectories)
- **Radiation** model (Baier-Katkov method) **TESTING NOW**
- **Pair production** model **NEXT YEAR**
- **Radiation** and **positron source examples** **NEXT YEAR**
- **Beam extraction example**: requires the implementation of beam dynamics in an accelerator **2024**



Thank you for attention!

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.);
G4LogicalVolume* crystalLogic = new G4LogicalVolume(crystalSolid,Silicon,"Crystal");
CrystalN1 = 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
    ChannelingFastSimModel* ChannelingModel = new ChannelingFastSimModel("ChannelingModel",RegionCh);
    //set the type of crystal planes
    G4String lattice = "(111)";
    //activate the channeling model
    ChannelingModel->Input(CrystalN1,lattice);
    //setting bending angle of the crystal planes (default is 0)
    BendingAngle = 0.905*mrad;
    ChannelingModel->GetCrystalData()->SetBendingAngle(BendingAngle);

    //activate radiation model (do it only when you want to take into account
    //radiation production in an oriented crystal; it takes a lot of computational power)
    ChannelingModel->RadiationModelActivate();
}
```

Get crystal region

Channeling FastSim model declaration

Physical volume

Model activation

Additional options

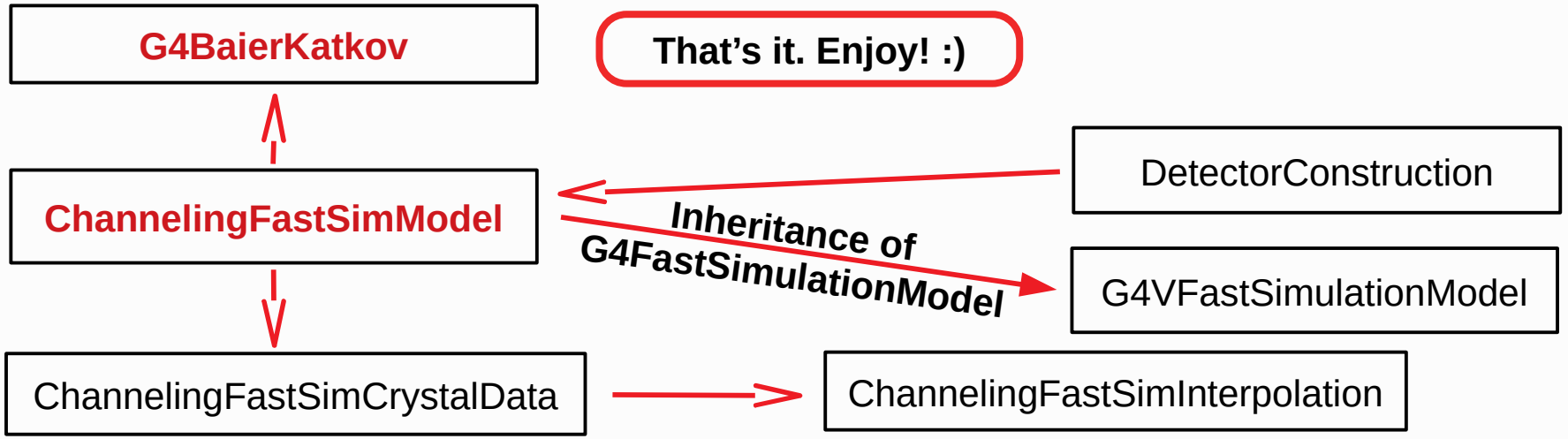
Radiation model activation

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 );
```



Physics list independent