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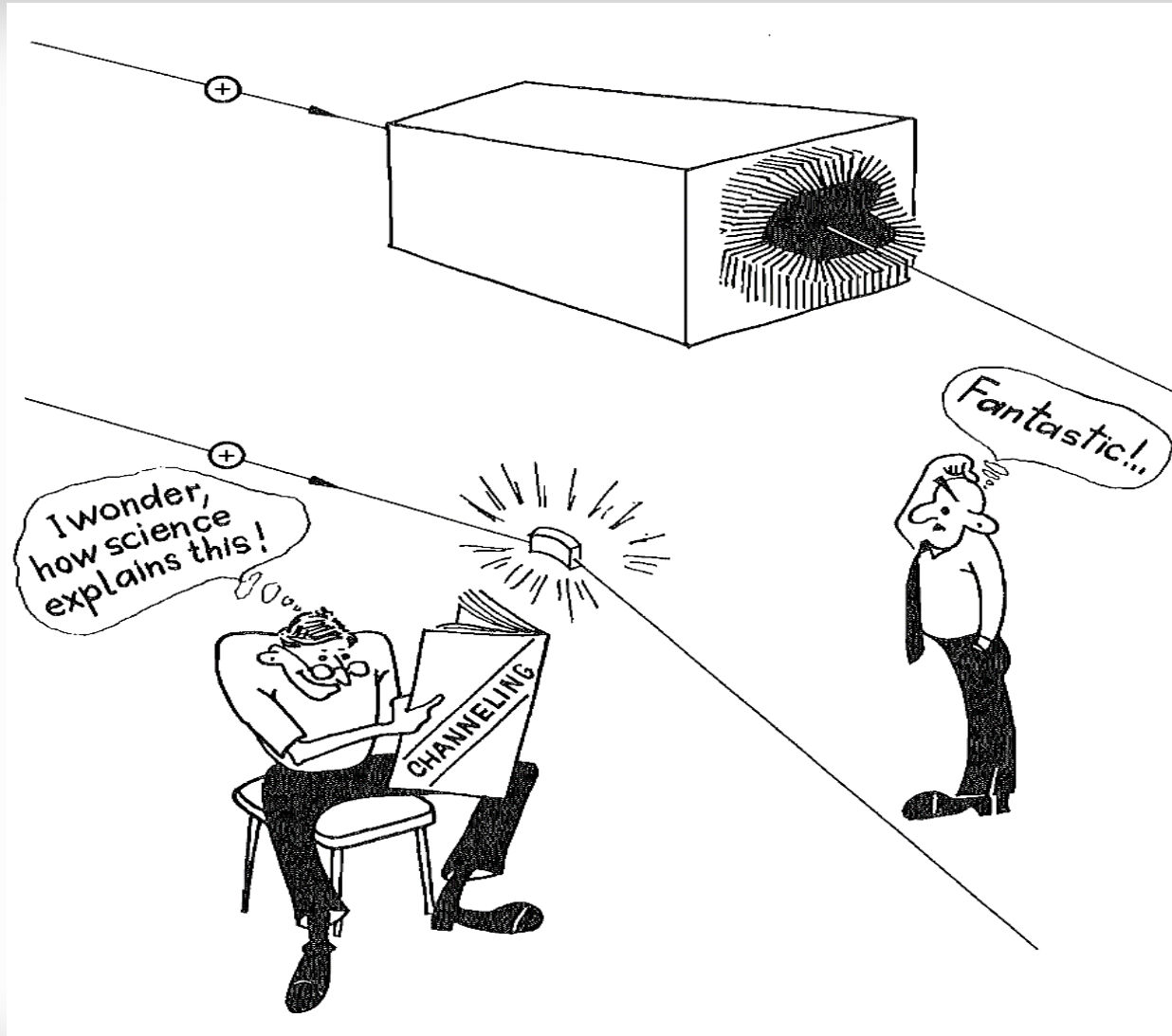
New Geant4 model of channeling in crystals and its potential applications

Dr. Alexei Sytov

27th Geant4 Collaboration Meeting

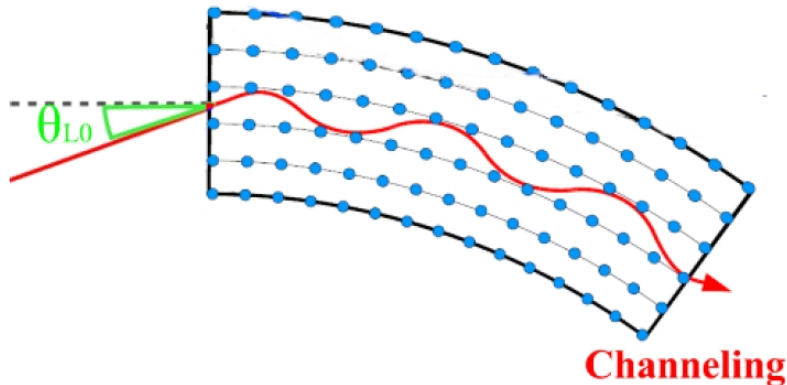
Rennes, 27/09/22

The world of the channeling effect and

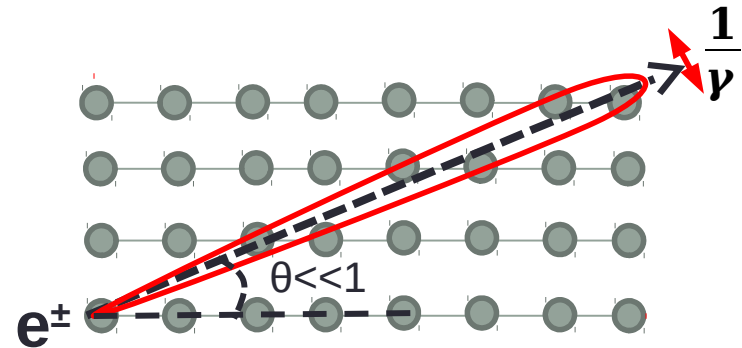


The idea: MC simulations of coherent effects in a crystal

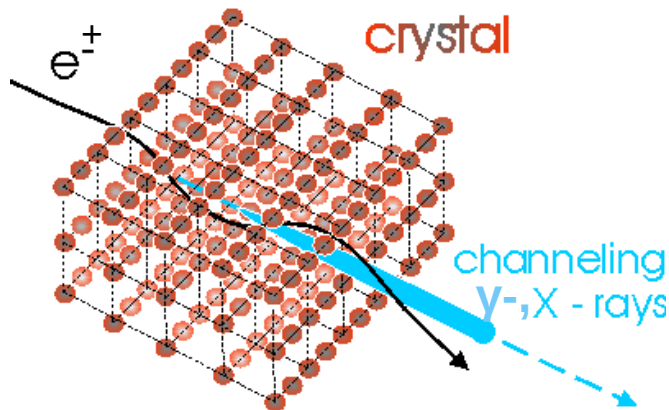
Channeling*



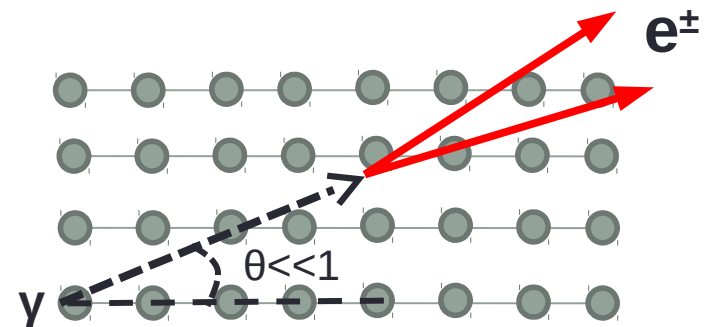
Coherent bremsstrahlung***



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)

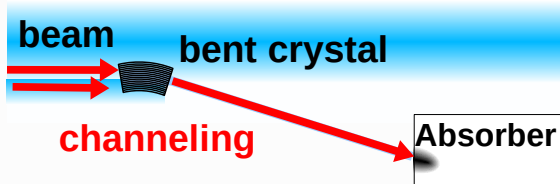
**M.A. Kumakhov, Phys. Lett. A 57(1), 17–18 (1976)

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

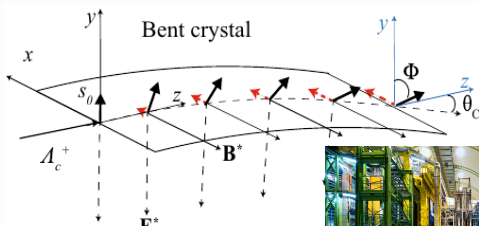
**** H. Überall, Phys. Rev. 103, 1055 (1956).

Applications*

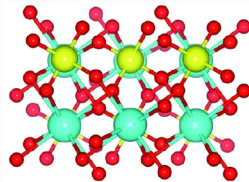
Crystal-based collimation
or beam extraction from an
accelerator



Measurement of dipole
magnetic and electric
moments of exotic particles



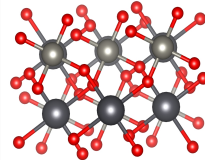
Ultrashort
crystalline
calorimeter



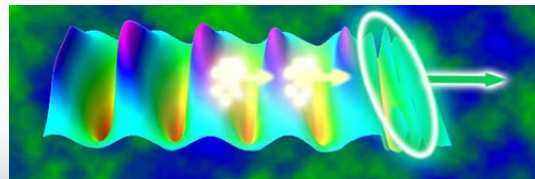
Gamma-ray
Space Telescope



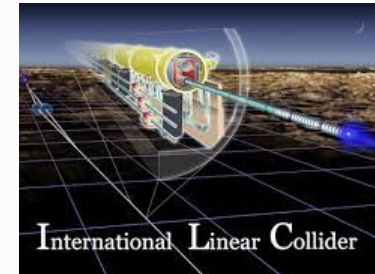
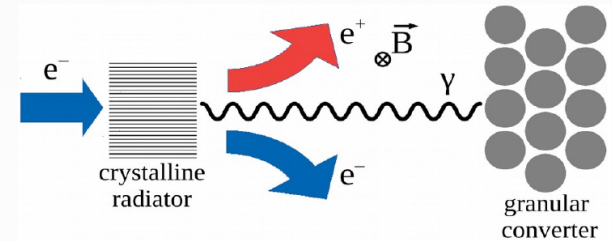
Oriented crystals



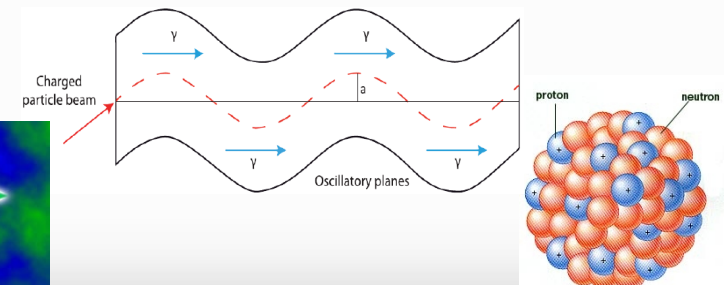
Plasma acceleration



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



X and γ-ray source for
nuclear and medical physics



Marie Skłodowska-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



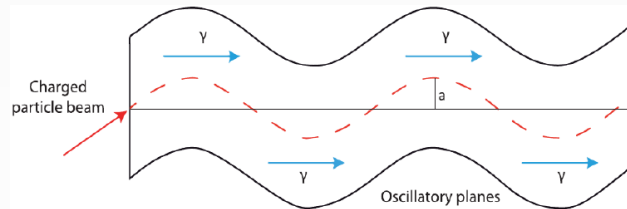
Location:

- 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)

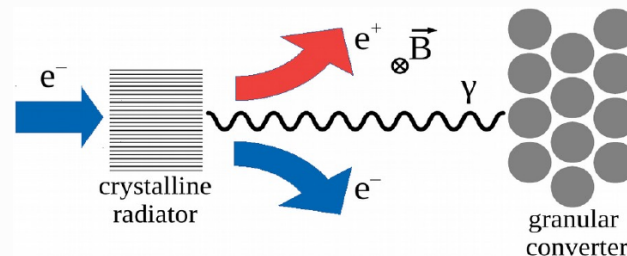
Marie Skłodowska-Curie Action Global Fellowships by A. Sytov in 2021-2024, Project TRILLION

Specific applications to implement into Geant4:

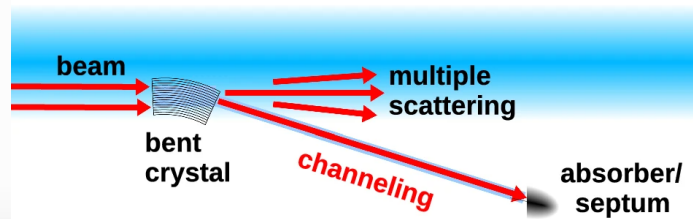
● **Crystalline source of hard X-ray and gamma radiation, crystalline undulator (CU).**



● **Crystal-based hybrid positron source** for both linear and circular e^+e^- colliders (ILC, FCC-ee*, KEKB etc.) as well as for **muon colliders**.



● **Crystalline deflector to extract a charged particle beam from an accelerator (electron synchrotron**, hadron collider) to supply fixed-target experiments by an intense low-emittance beam.**



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

**A. Sytov et al. Eur. Phys. J. C 82, 197 (2022)

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**

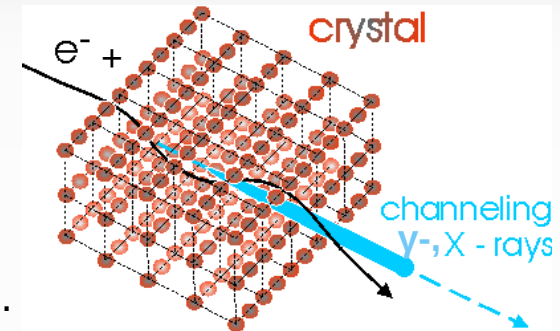
Baier-Katkov formula:

integration is made over the classical trajectory

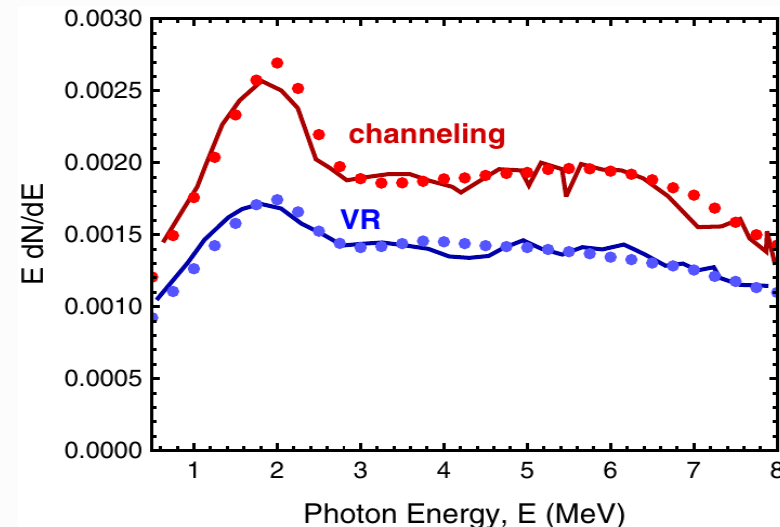
$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{[(E^2 + E'^2)(v_1 v_2 - 1) + \omega^2 / \gamma^2]}{2E'^2} e^{-ik'(x_1 - x_2)}$$

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)

Our project MIRACLE, no. HP10BIW7VR Cineca ISCRA Class B National Italian project



MIRACLE

Medical physics and RAdiation in Crystals simuLation with gEant4

Main goal: to supply **Italian Geant4 community** and their international collaborators by CINECA HPC resources necessary to accomplish **MC_INFN** and **TRILLION** projects.

25/10/2021 - 25/10/2022

Marconi 100: 0.992 Mh for 1 year

Galileo 100: 2.4 Mh for 1 year

Italian organizations involved

- INFN Sezione di Catania
- INFN Sezione di Ferrara
- INFN Laboratori Nazionali del Sud
- INFN Napoli
- INFN Roma1
- Istituto Superiore di Sanità
- University of Messina
- University of Napoli

PI A. Sytov

I can add additional collaborators,
ask me!

Foreign organizations involved

- ELI-Beamlines, Institute of Physics, (FZU), Czech Academy of Sciences
- Institute for Nuclear Problems, Belarus
- University of Surrey



Progress of channeling physics implementation into Geant4



GEANT4
A SIMULATION TOOLKIT

Status of channeling 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

```
93
94
95
96
97
98
99
100
101
102
103
104
105
106
107
108
109
110
111
112
113
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

Solution: 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  //.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....
82
83  G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
84  {
85
86
87
88
89
90
91
92
93
94
95
96
97
98
99
100
101
102  }
103
104  //.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....
105
106  void TestModel::DoIt(const G4FastTrack& fastTrack,
107                      G4FastStep& fastStep)
108  {
```

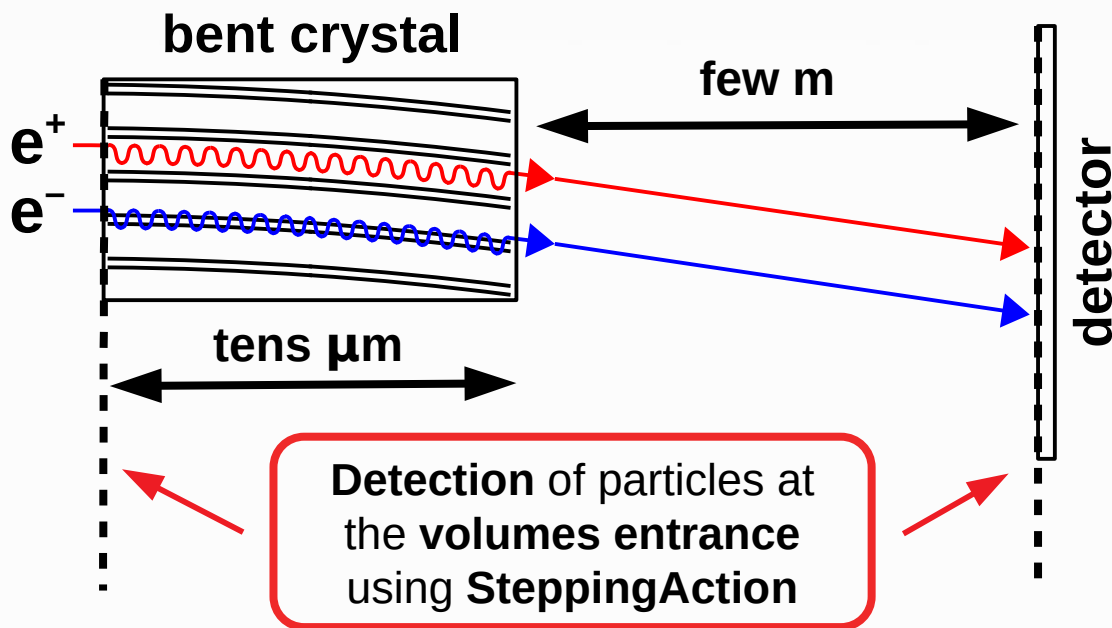
Insert particles for which
the model is applicable

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 Mikrotрон MAMI



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

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

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



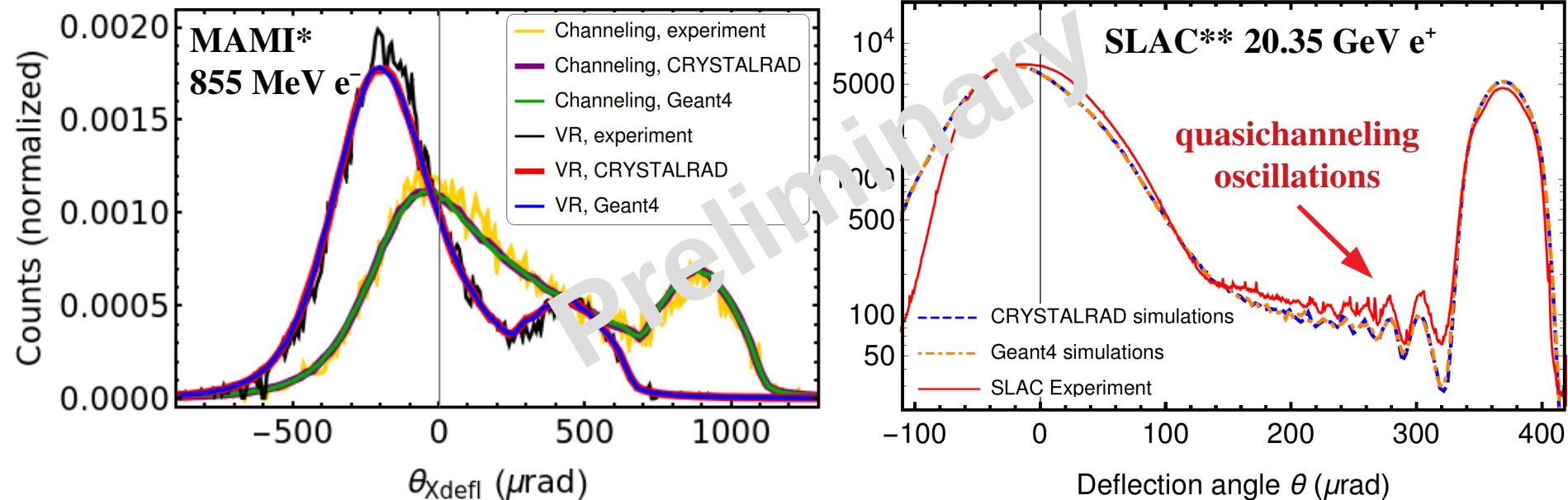
*A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

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

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



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)

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);
}
```

Get crystal region

Channeling FastSim
model declaration

Physical volume

Model activation

Additional options
if necessary

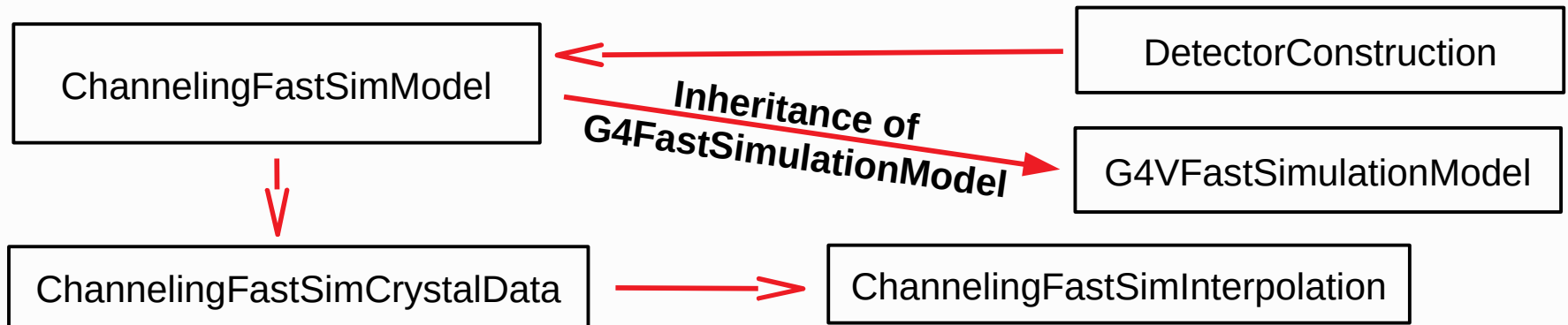
How to use the Geant4 channeling model in your example?

● 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 );
```

That's it. Enjoy! :)



Physics list independent

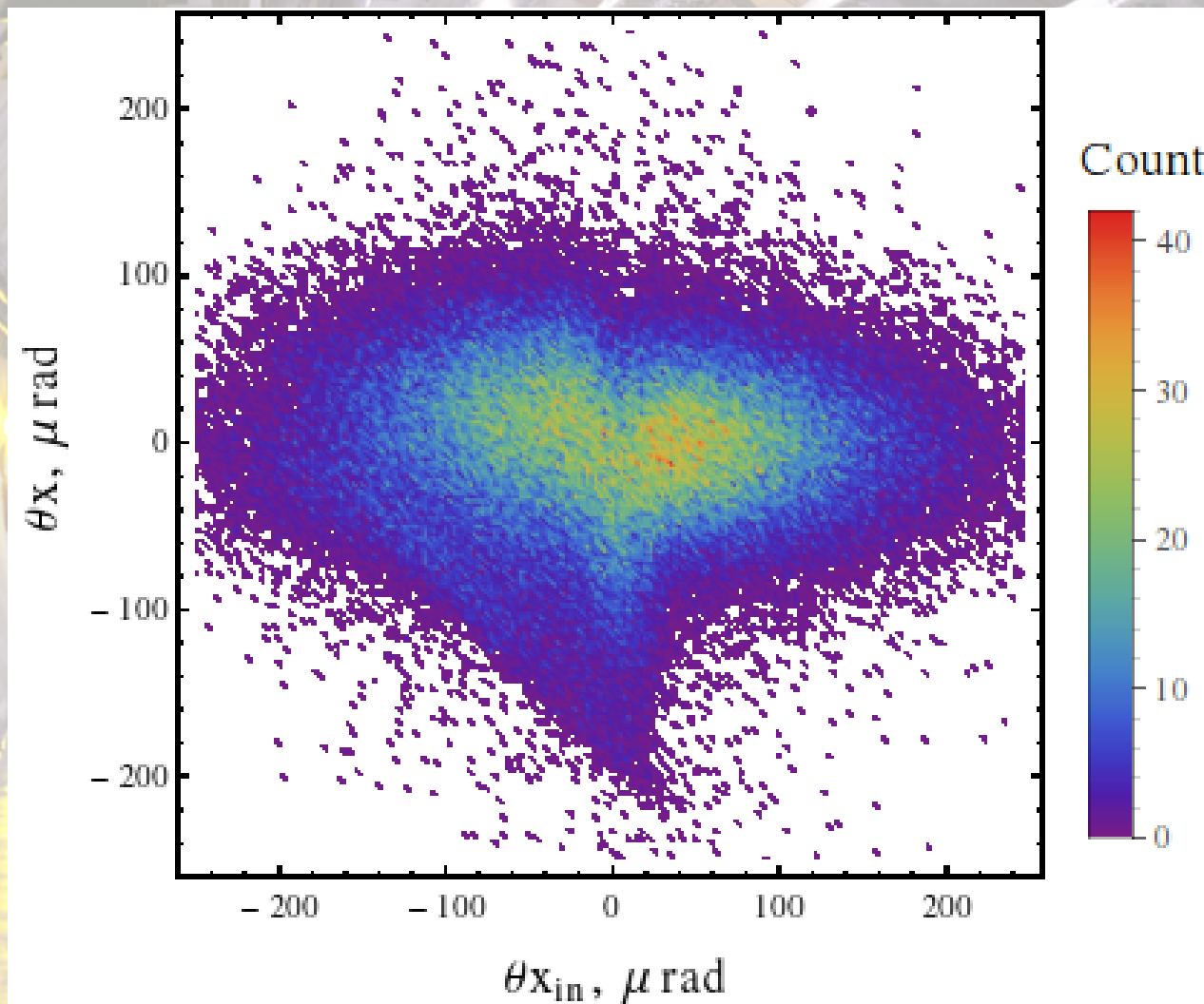
New channeling model implementation into Geant4

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) **IN PROGRESS 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**

*More details about the radiation model at VI Geant4 International User Conference at Napoli in **my talk** on 25/10/2022 at 15.25:
<https://agenda.infn.it/event/21084/contributions/178018/>



Thank you for attention!