INFN
Istituto Nazionale di Fisica Nucleare

European Commission

Trillion

New examples for transport in crystals

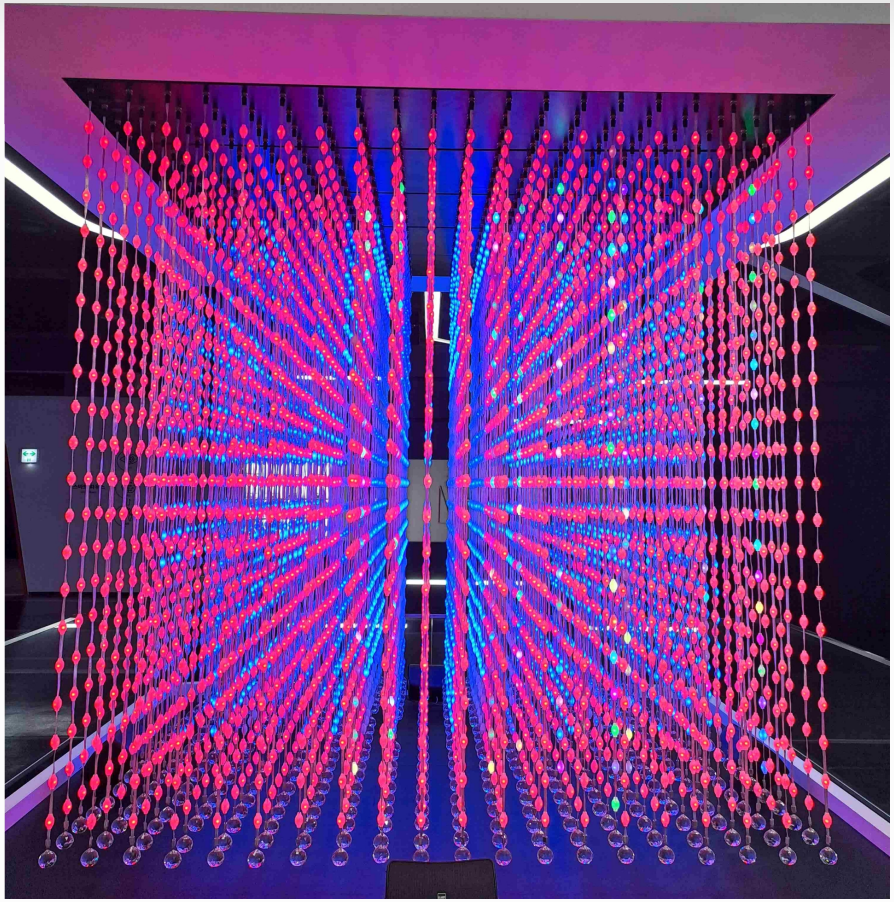
Marie Curie Global Fellowships, Project TRILLION GA n. 101032975

Dr. Alexei Sytov

In close collaboration with Dr. Gianfranco Paternò

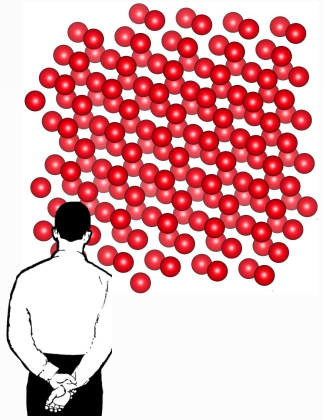
Geant4 EM physics meeting 09/07/2024

How an oriented crystal looks like

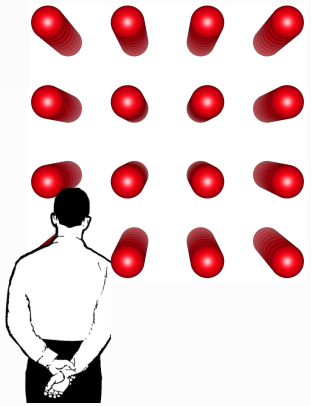


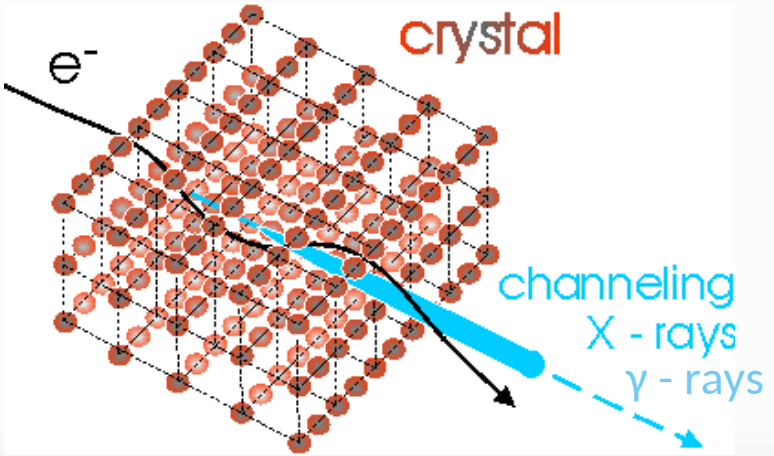
from National Science Museum, Daejeon, Korea

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:

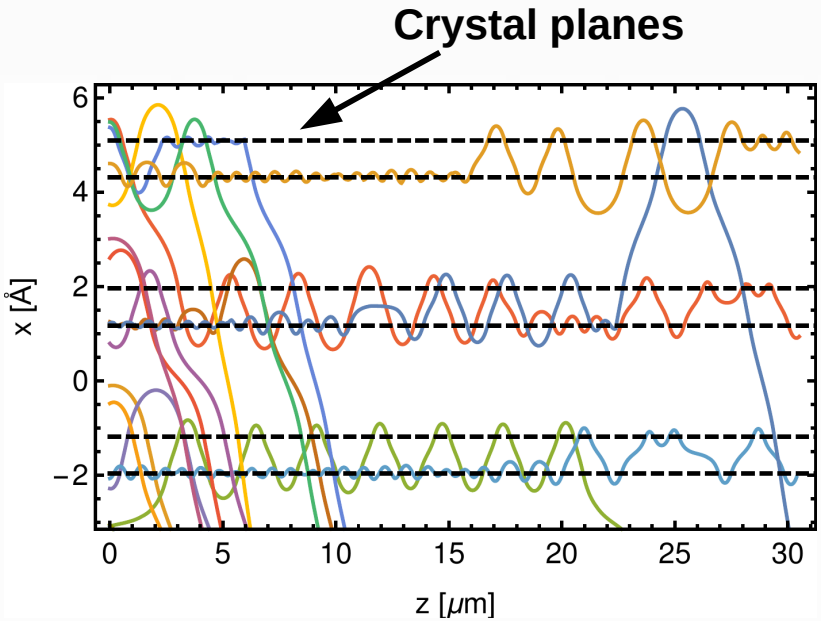
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

Location:

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

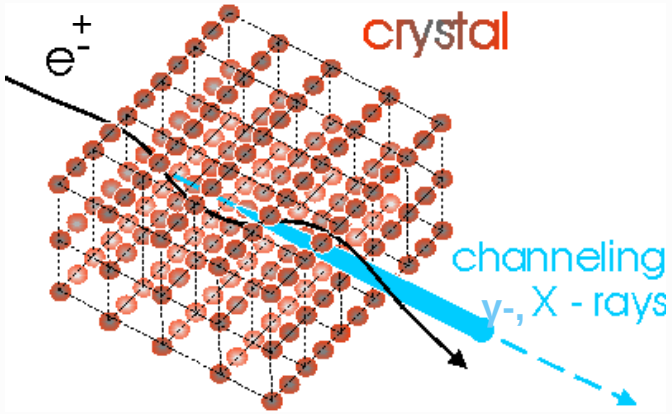


channeling*

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

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

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. 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

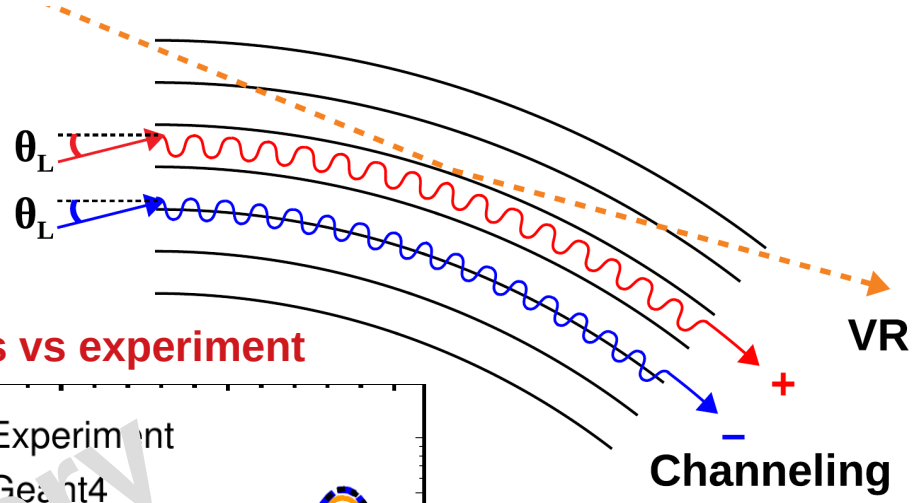
Please cite our papers if you use our model:

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

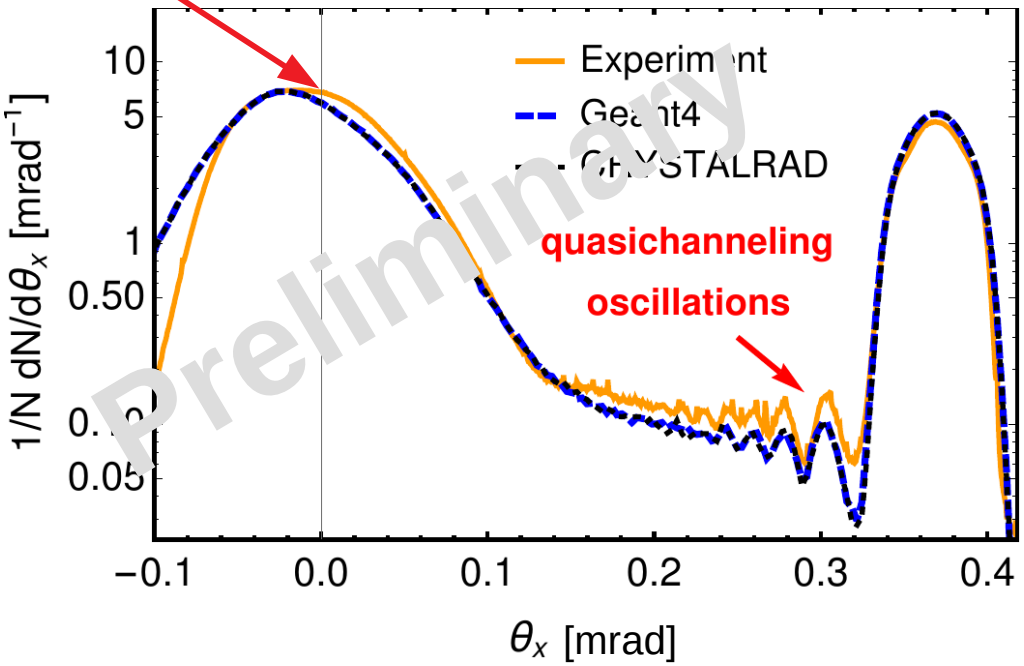
60 µm thick bent crystal



volume reflection (VR)

channeling

Geant simulations vs experiment



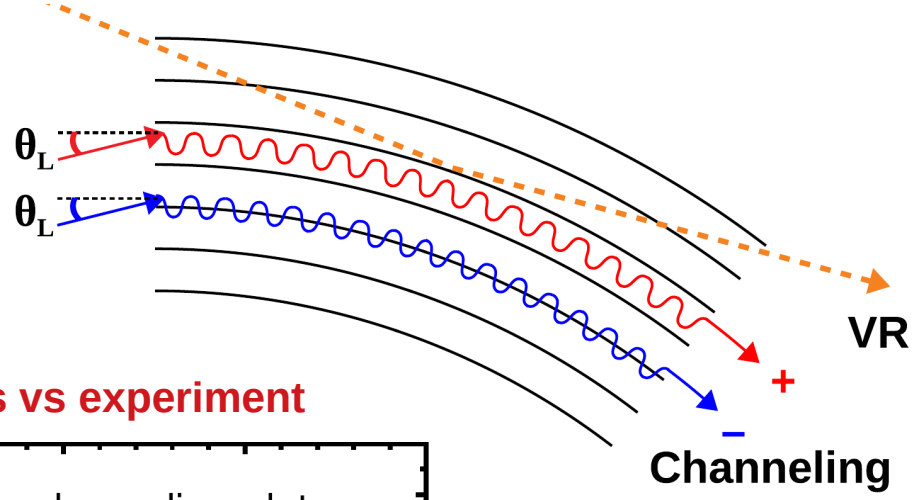
To be submitted for publication soon

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

Geant4 channeling model validation: beam deflection by a bent crystal

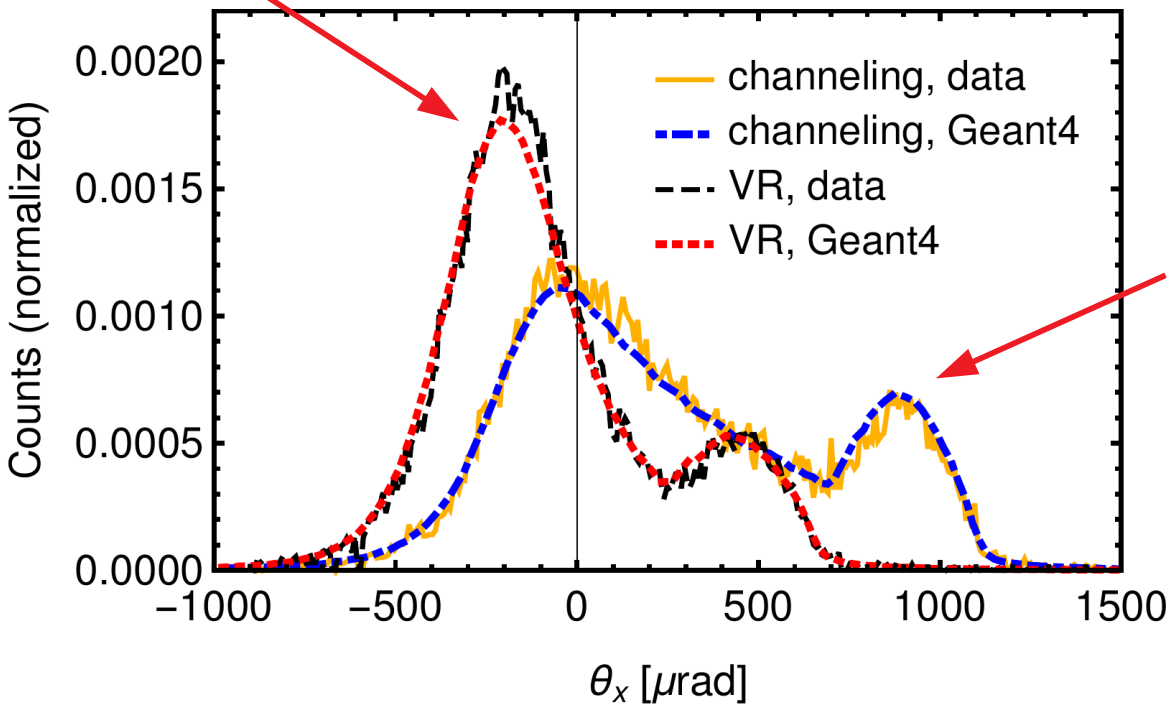
855 MeV electrons

15 µm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



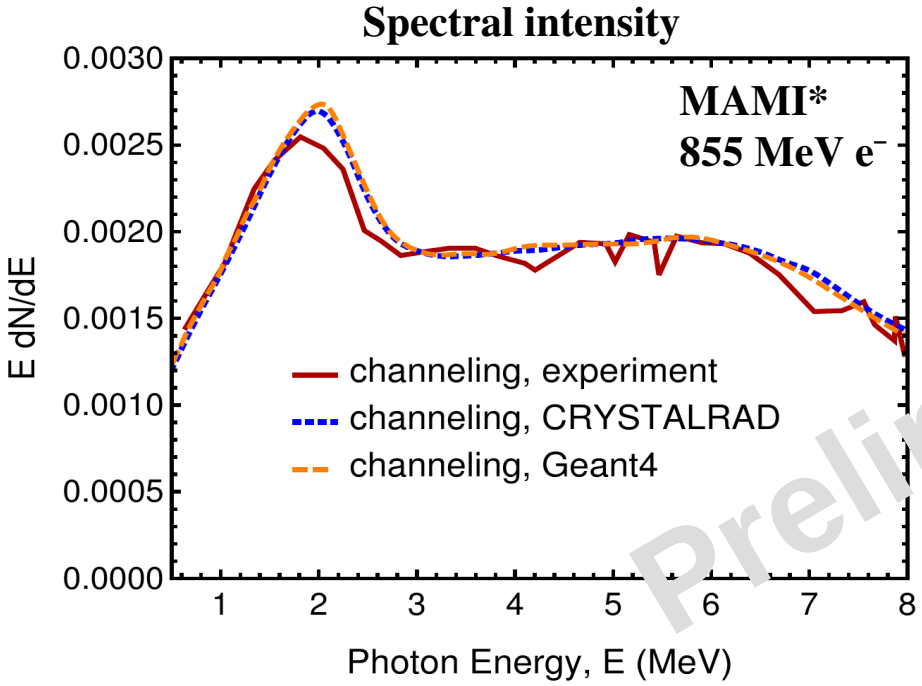
channeling

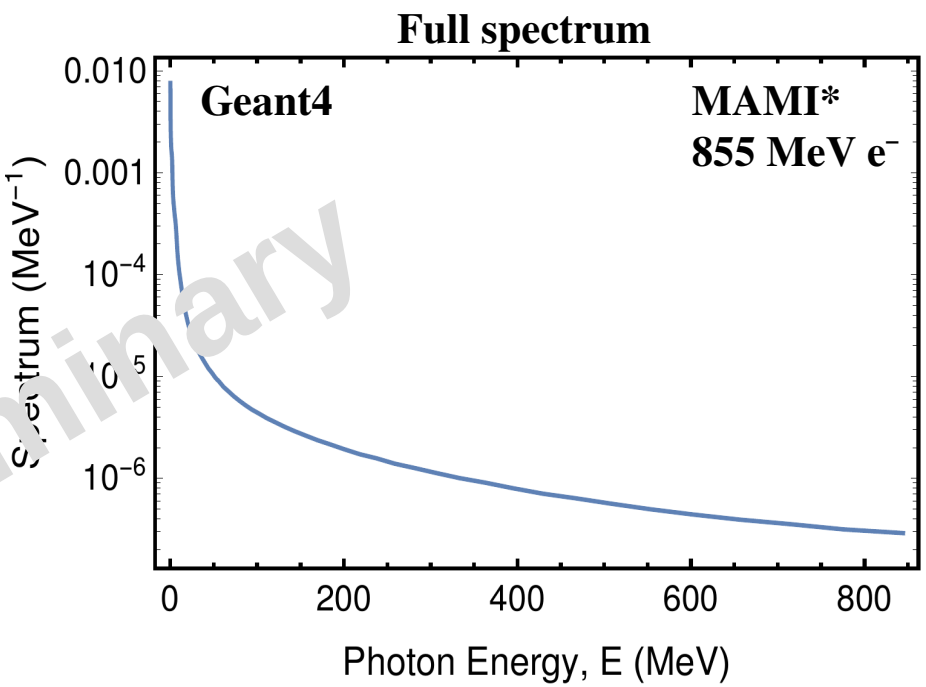
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

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



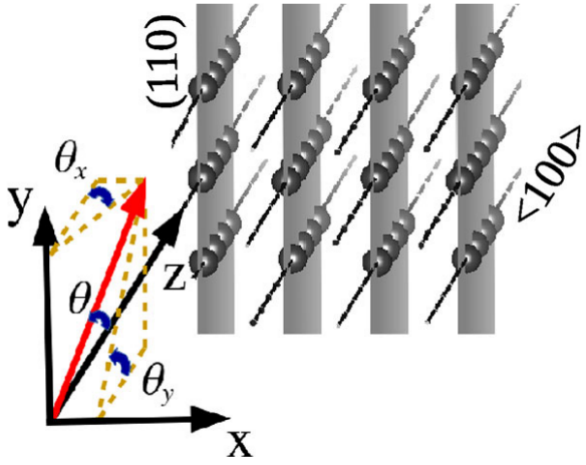


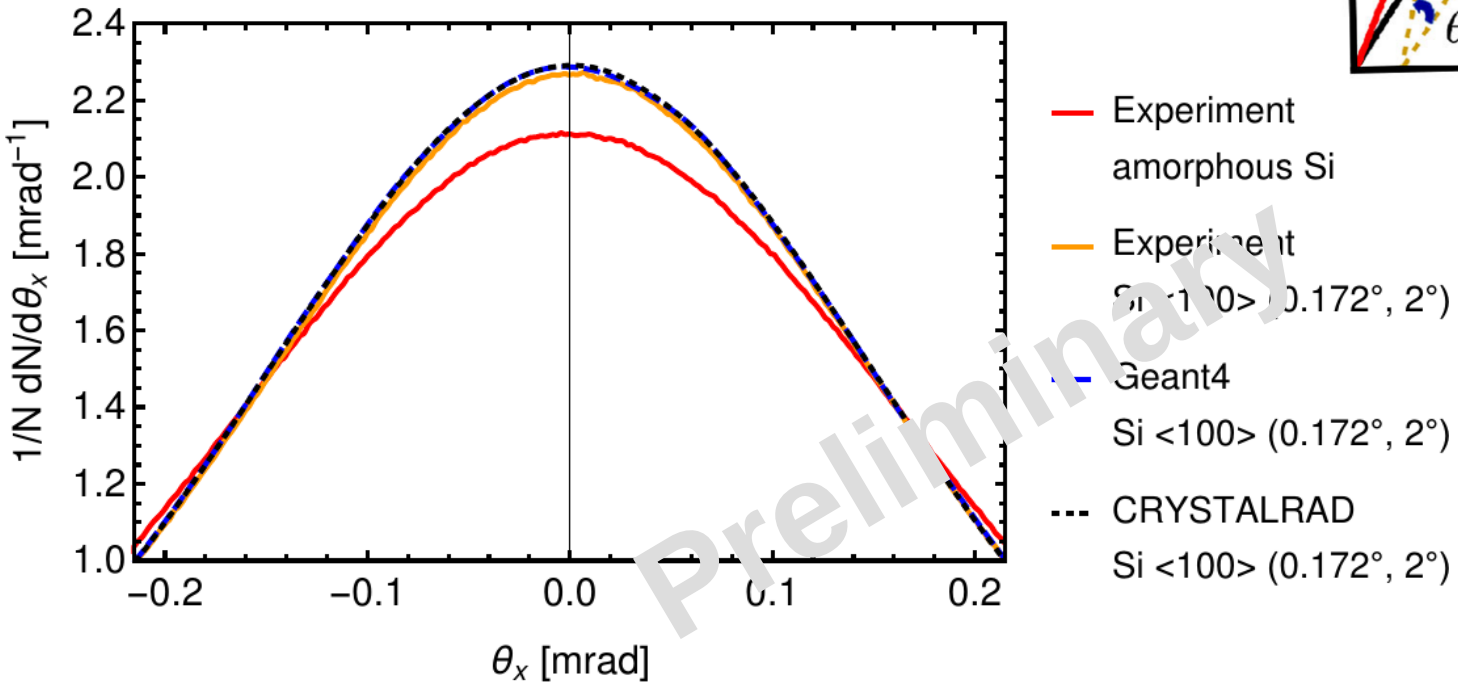
To be submitted for publication soon

*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!

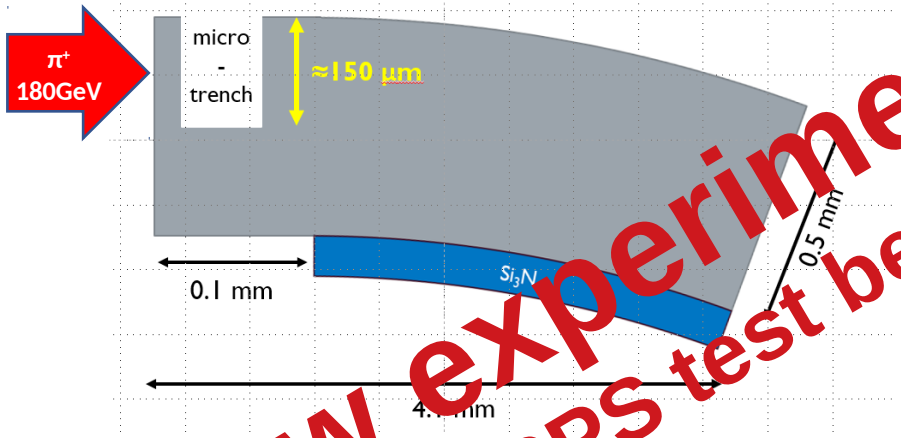




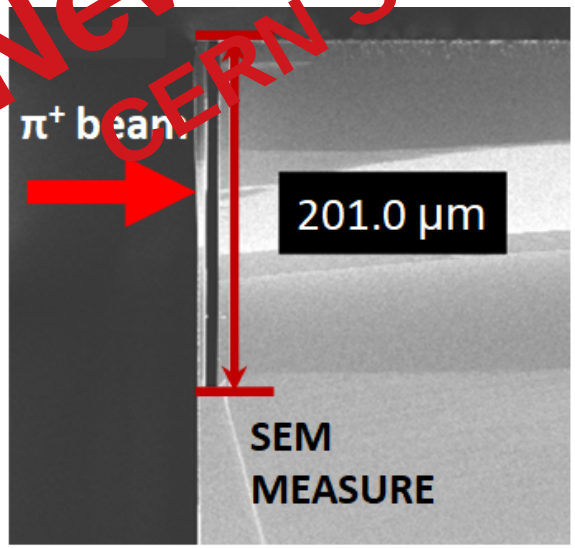
To be submitted for publication soon

*A. Mazzolari, A. Sytov et al. Eur. Phys. J. C 80, 63 (2020)

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



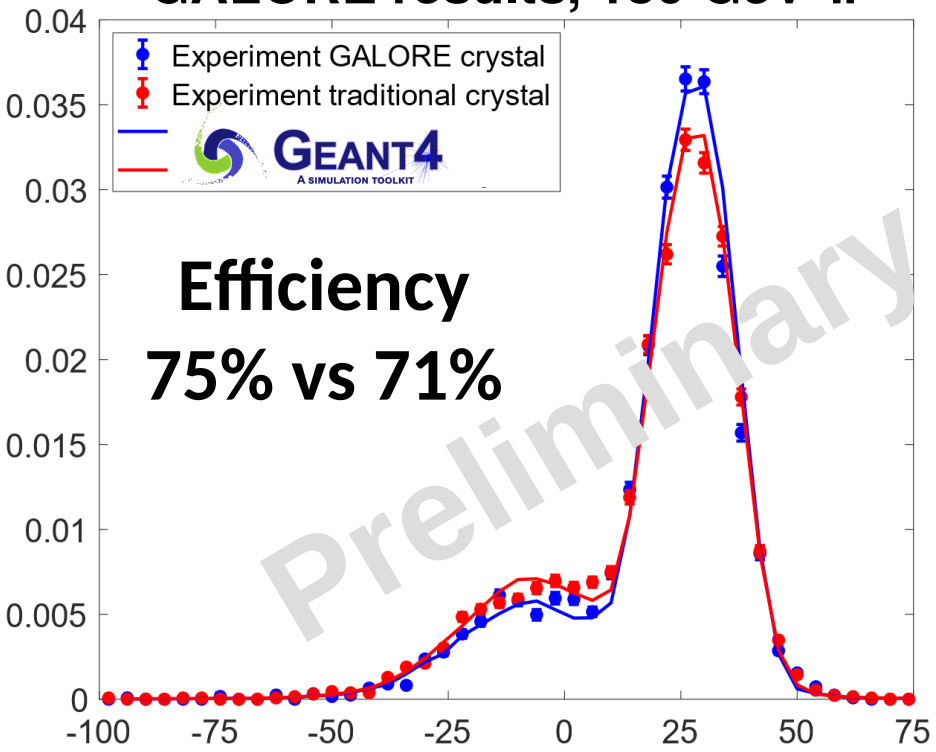
New experiment
CERN SPS test beam



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).

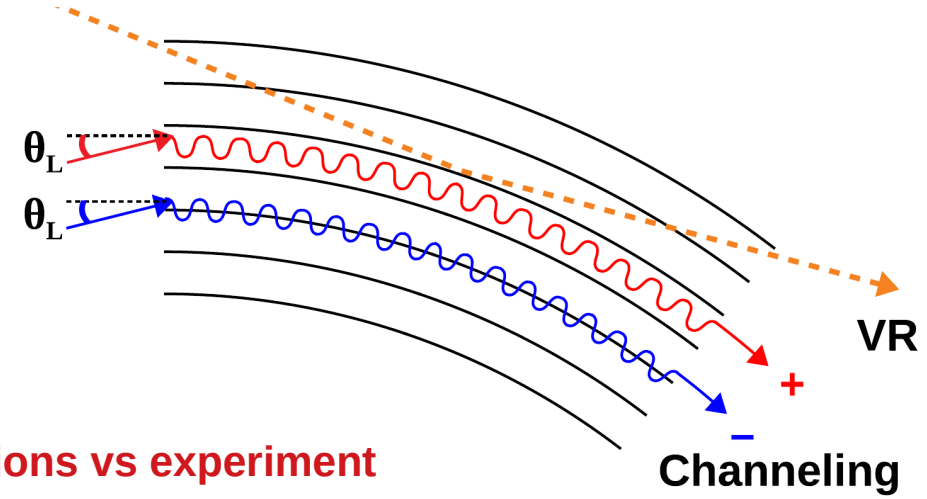
*V.V. Tikhomirov JINST 2 P08006 (2007)

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

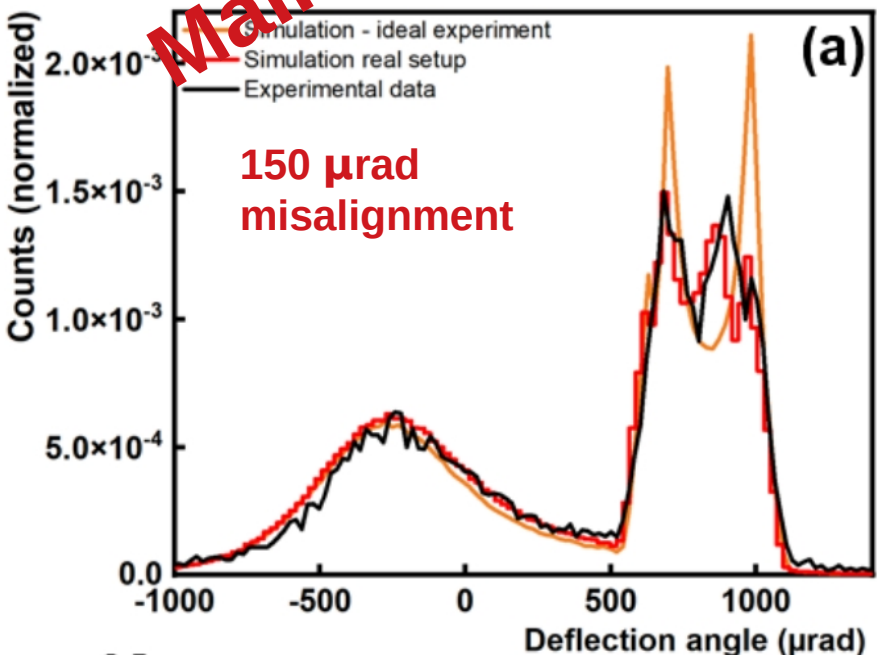
530 MeV positrons

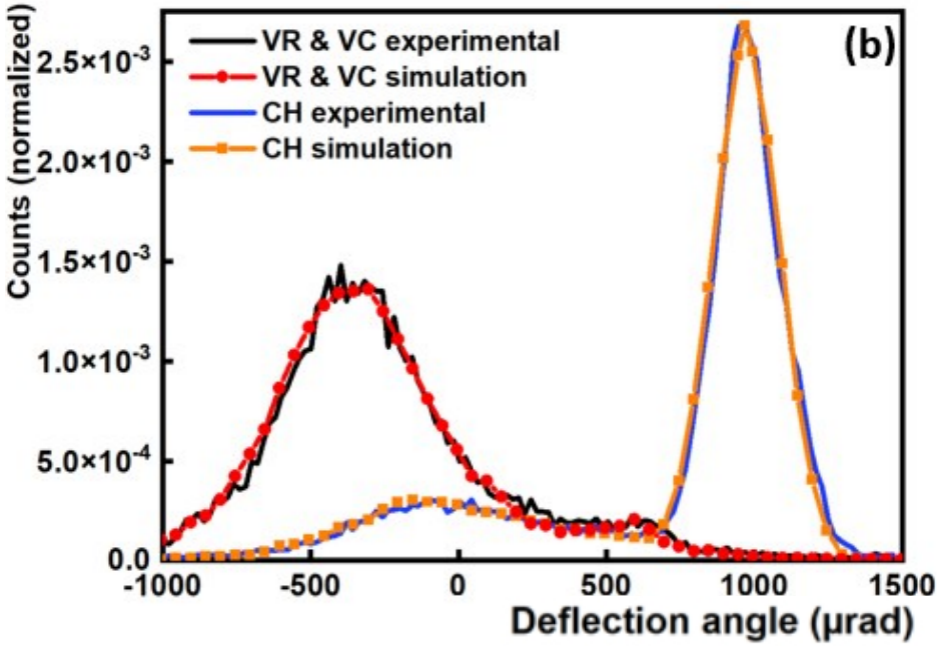
30 µm thick bent crystal

New experiment Mainz Mikrotron 2024

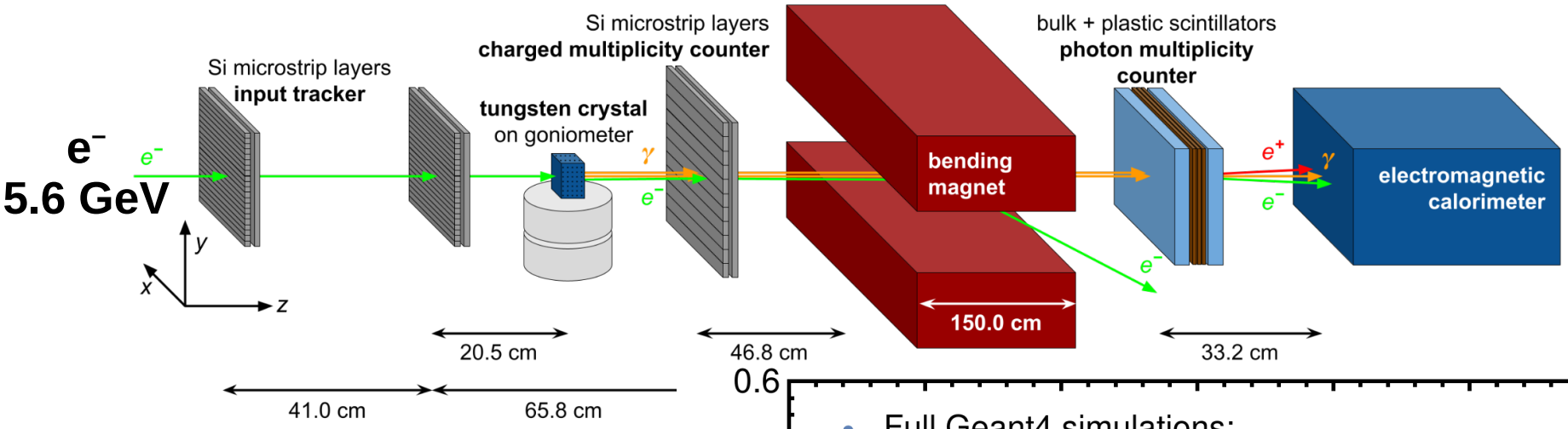


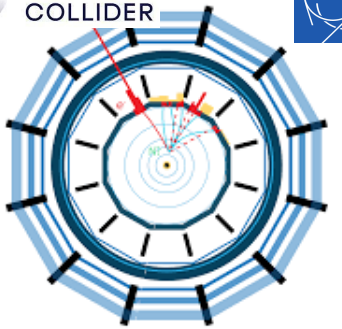
Geant simulations vs experiment

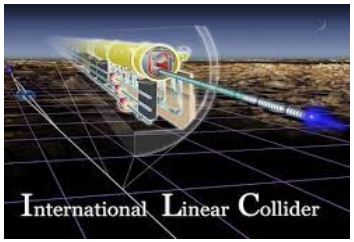


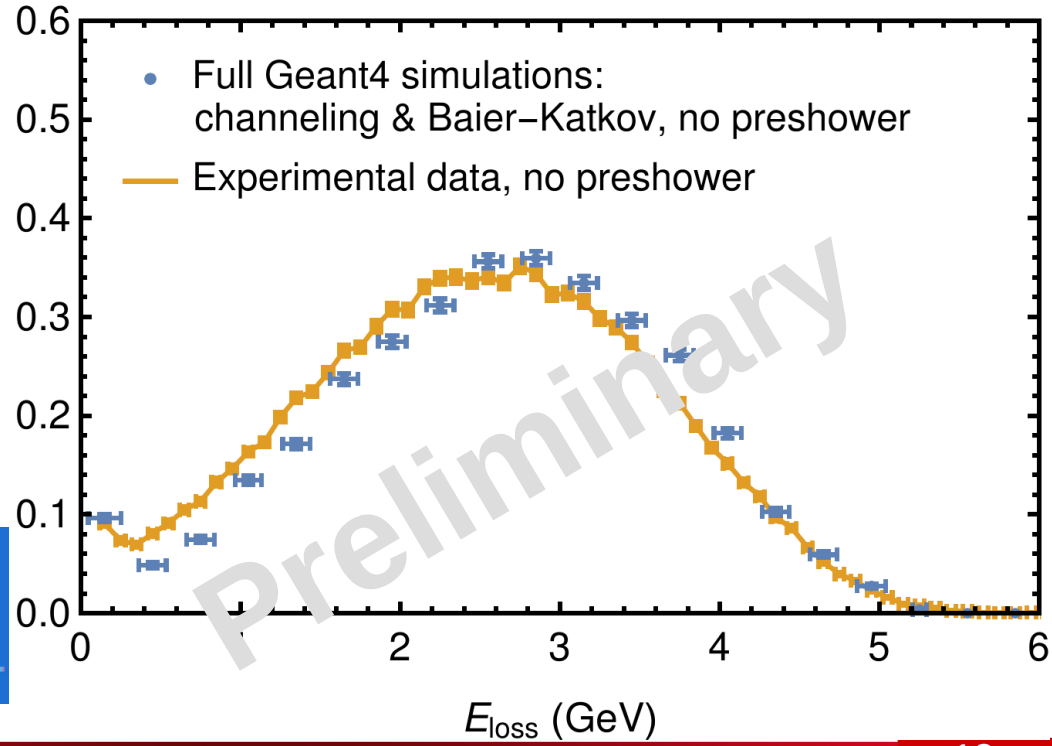


Full Geant4 simulations of the DESY experiment* for the FCC-ee positron source project









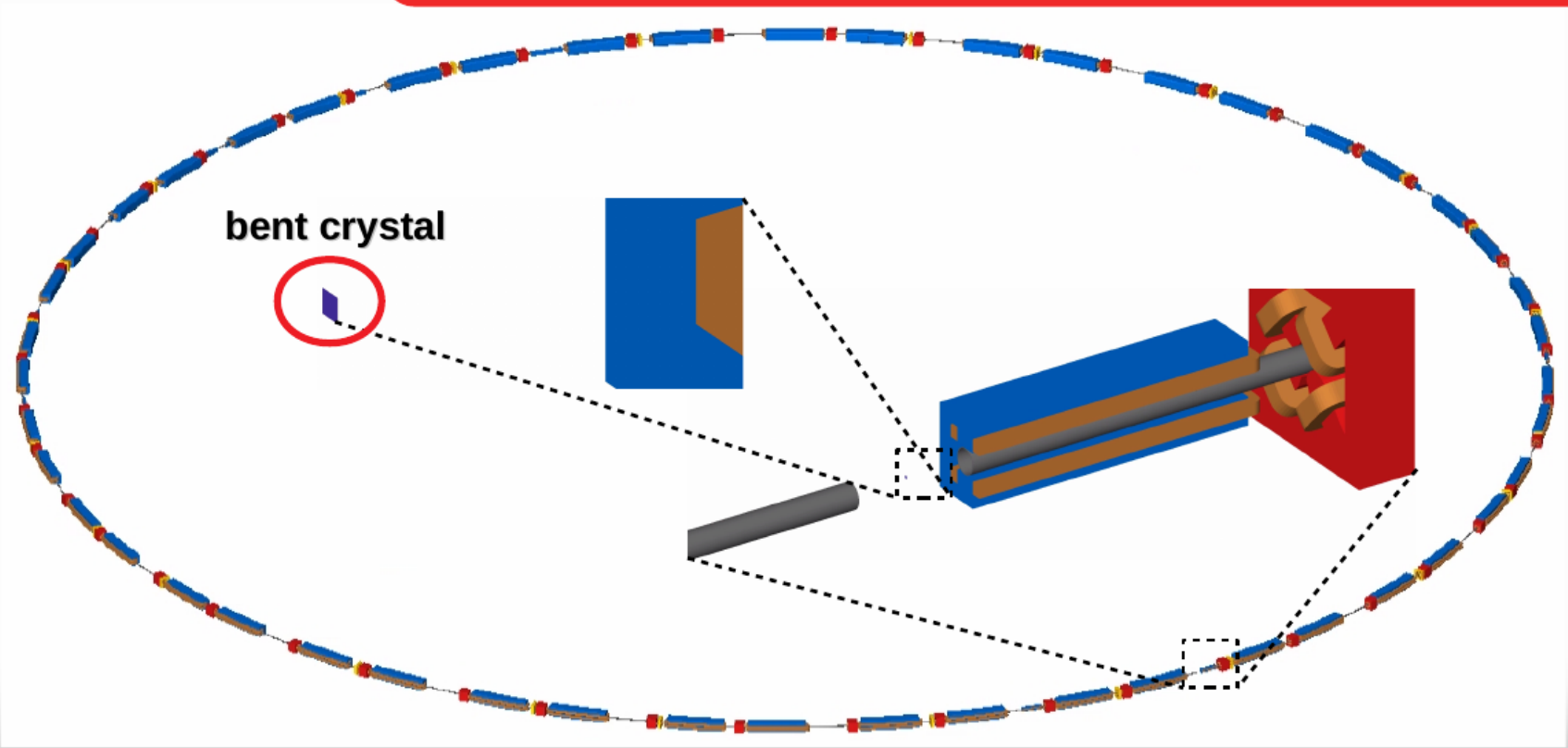
***Intense positron source Based On Oriented crySTals* - e+BOOST**
(PI L. Bandiera)
PRIN2022-2022Y87K7X
Financed by Italian Ministry of University and Research - PRIN project

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

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.



Implementation of a new component and a new physics list

```cpp
#include "BDSIMClass.hh" // bdsim interface

#include "CrystalDeflector.hh"
#include "CrystalDeflectorConstructor.hh"

#include "FTFP_BERT.hh"
#include "G4FastSimulationPhysics.hh"
#include "G4StepLimiterPhysics.hh"
#include <iostream>

int main(int argc, char** argv)
{
  // construct an instance of bdsim
  BDSIM* bds = new BDSIM();

  // Physics list
  G4VModularPhysicsList* physicsList = new FTFP_BERT;
  // -- Create helper tool, used to activate the fast simulation:
  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 );
  physicsList->RegisterPhysics(new G4StepLimiterPhysics());
  bds->RegisterUserPhysicsList(physicsList);

  // register a custom component by name udipole with a user-provided constructor
  // BDSIM will delete the constructor at the end.
  bds->RegisterUserComponent("crystaldeflector", new CrystalDeflectorConstructor());

  // construct geometry and physics
  bds->Initialise(argc, argv);
  if (!bds->Initialised()) // check if there was a problem.
    {std::cout << "Intialisation failed" << std::endl; return 1;}

  bds->BeamOn(); // run the simulation
  delete bds;    // clean up
  return 0;      // exit nicely
}
```

CrystalDeflectorConstructor.cc

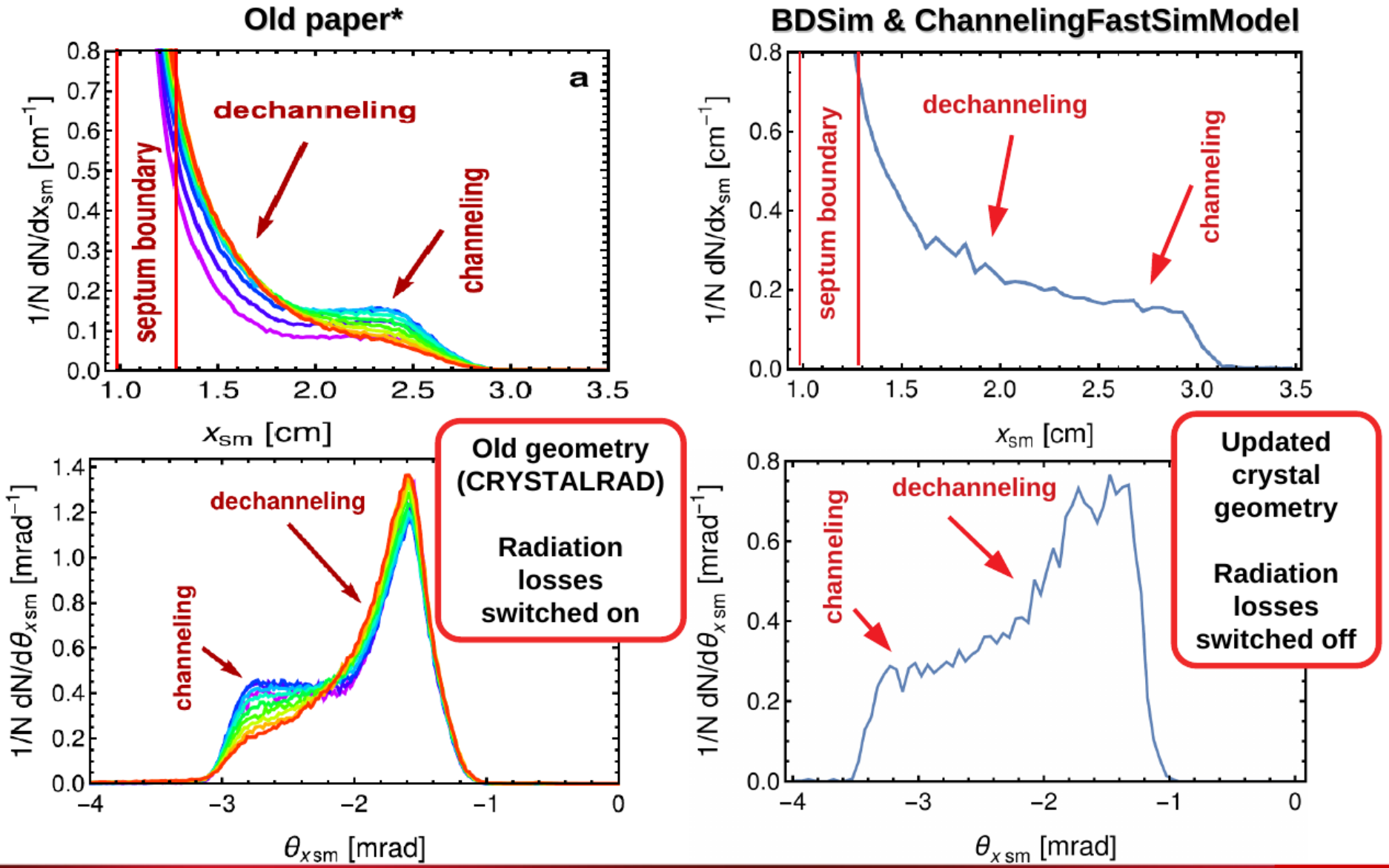
```cpp
BDSAcceleratorComponent* crystal = new CrystalDeflector(element->name,
                                                        element->l*CLHEP::m,
                                                        element->xsize*CLHEP::m,
                                                        element->ysize*CLHEP::m,
                                                        element->materialThickness*CLHEP::m,
                                                        element->axisX,
                                                        element->axisY,
                                                        element->axisZ,
                                                        horizontalWidth*CLHEP::m,
                                                        bendingAngle,
                                                        material,
                                                        vacuumMaterial,
                                                        crystalLattice,
                                                        region,
                                                        colour,
                                                        radiationModel);
```

```
D12H: drift, l=0.4125;
CR1: usercomponent, userTypeName="crystaldeflector",
l=0.4125, xsize=1*cm, ysize=1*cm,
materialThickness=0.175*mm, offsetX=-1.126046*cm,
offsetY=0*mm, axisX=0.000, axisY = -0.00097, axisZ = 0.,
horizontalWidth=1*m,  material="G4_Si",
vacuumMaterial="vacuum",
userParameters="crystalRegion:crystal1
crystalBendingAngle:0.00175 crystalLattice:(111)
colour:decapole radiationModel:false"; dump1: dump,
l=1*mm, horizontalWidth=4*cm,
apertureType="rectangular",offsetX=2.98*cm;
D18: drift, l=0.495;
```

CrystalDeflectorConstructor.cc

```
void CrystalDeflector::BuildCrystal()
{
    //build crystal solid
    G4Box* crystalSolid = new G4Box(name + "_crystal_solid",
                                    crystalXSize * 0.5,
                                    crystalYSize * 0.5,
                                    crystalMaterialThickness * 0.5);
    RegisterSolid(crystalSolid); // for deletion by bdsim

    // make a logical volume for the crystal
    G4LogicalVolume* crystalLV = new G4LogicalVolume(crystalSolid,
                                                     crystalMaterial,
                                                     name + "_crystal_lv");

    // visualisation attributes - make it nicely visible
    G4VisAttributes* crystalVis = new G4VisAttributes(*BDSColours::Instance()->GetColour(crystalcolour));
    crystalVis->SetVisibility(true);
    crystalLV->SetVisAttributes(crystalVis);
    RegisterVisAttributes(crystalVis);// for deletion by bdsim
    RegisterLogicalVolume(crystalLV); // for deletion by bdsim

    G4RotationMatrix* crystalRM = new G4RotationMatrix();
    crystalRM->rotateX(crystalAxisX);
    crystalRM->rotateY(crystalAxisY);
    crystalRM->rotateZ(crystalAxisZ);
    RegisterRotationMatrix(crystalRM); // for deletion by bdsim
    G4double crystalZPos = 0*CLHEP::cm;
    G4ThreeVector crystalPos = G4ThreeVector(0,0, crystalZPos);

    //physical volume
    auto crystalPV = new G4PVPlacement(crystalRM,
                                       crystalPos,
                                       crystalLV,
                                       name + "_crystal",
                                       containerLogicalVolume,
                                       false,
                                       0,
                                       checkOverlaps);
    RegisterPhysicalVolume(crystalPV); // for deletion by bdsim

    G4Region* crystalRegion = new G4Region(crystalRegionName);
    crystalRegion->AddRootLogicalVolume(crystalLV);

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

    if(crystalRadiationModel){ChannelingModel->RadiationModelActivate();}
```

Crystal-based extraction: simulation results distributions at the septum magnet entrance



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

Approximate list of examples to include in Geant4 in 2024

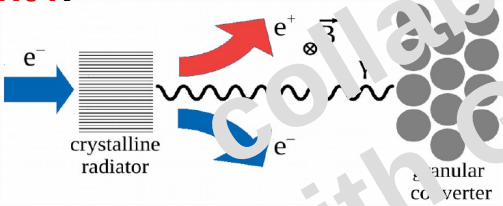
Examples:

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

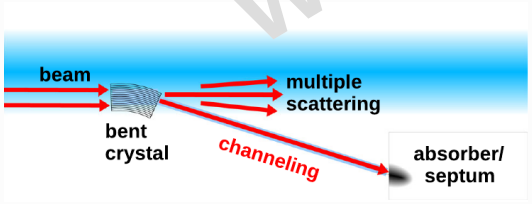
- Very **easy example** to demonstrate basic commands to include the channeling model in DetectorConstruction (no input/output) — **In test folder**
- **Complex example** including both channeling and radiation model, input with macro commands, root output and full spectrum of options — **Almost ready**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

Specific applications to implement into Geant4:

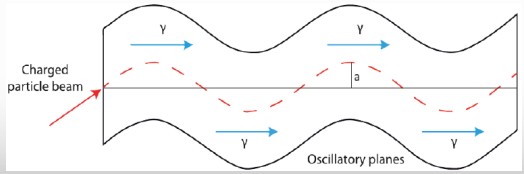
- **Crystal-based hybrid positron source for FCC-ee** — **Almost ready**



- **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**



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

Thank you! 감사합니다 !