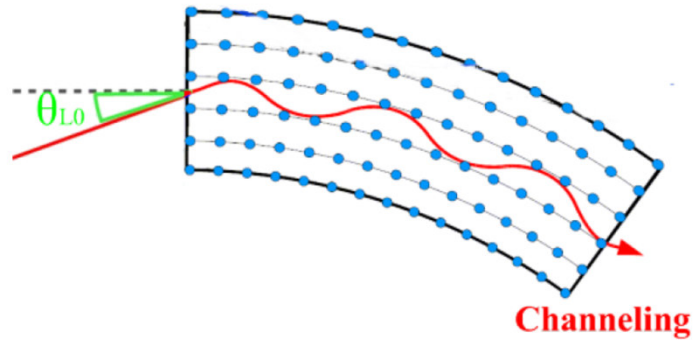


# Geant4 code for the optimization of Positron Sources based on oriented crystals

Gianfranco Paternò  
INFN – Ferrara division

# Coherent effects in a crystal

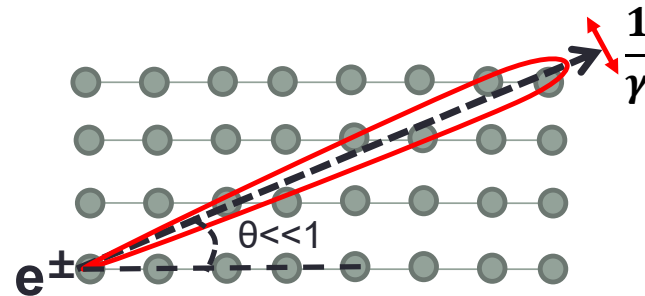
Channeling\*



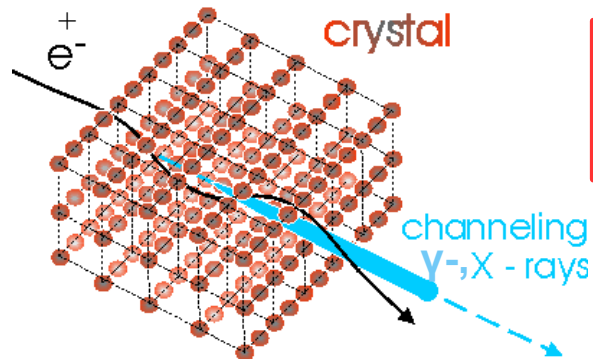
Energies:  
MeV - TeV

Equivalent  
magnetic  
field: more  
than 100 T

Coherent bremsstrahlung\*\*\*

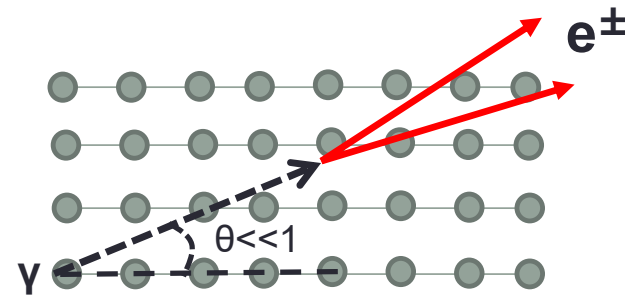


Channeling radiation\*\*



Planar/  
Axial field  
 $10^9/10^{11}$  V/cm

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)

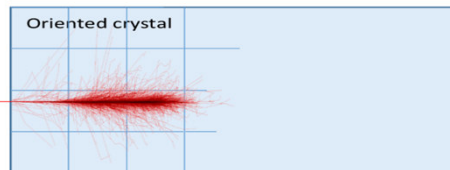
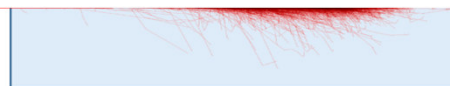
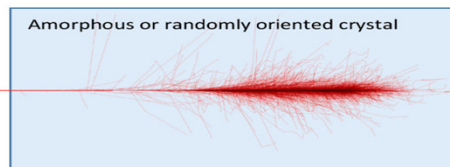
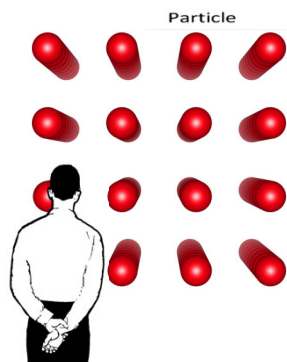
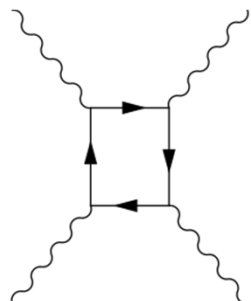
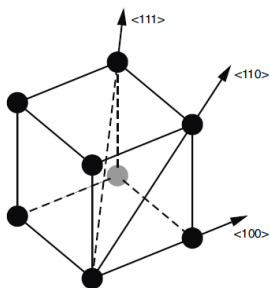
\*\*\*B. Ferretti, Nuovo Cimento 7, 118 (1950); M. Ter-Mikaelian, Sov. Phys. JETP 25, 296 (1953).

# Electromagnetic shower acceleration

**Axial field  
 $10^{11}$  V/cm**



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

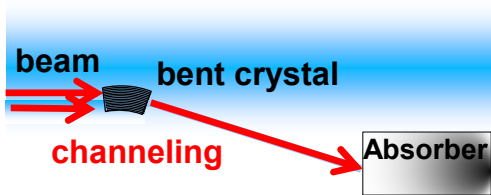


**The radiation intensity and the pair production cross-section drastically increase in oriented crystals!**

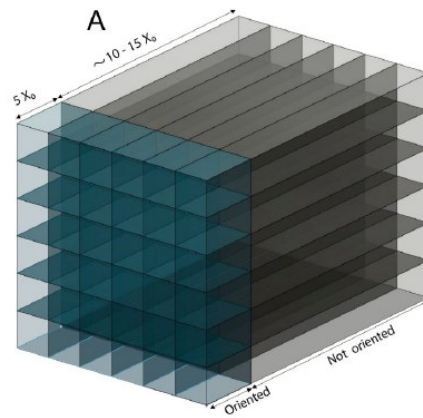
**Shower development in the field of axes is accelerated. The radiation length is considerably reduced\*.**

# Some of the possible applications of oriented crystals

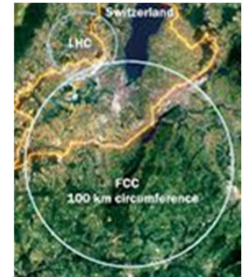
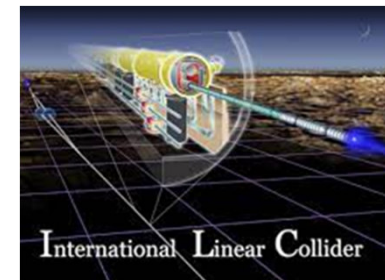
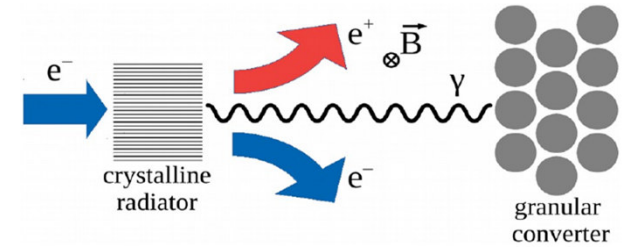
Crystal-based collimation or beam extraction from an accelerator



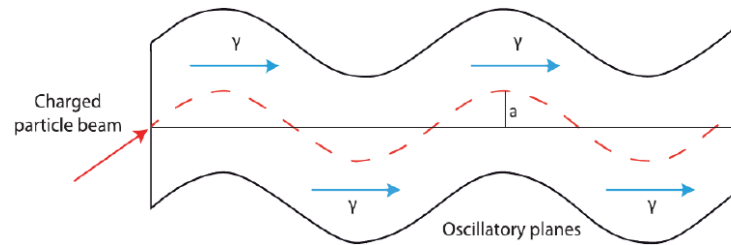
Compact Oriented Calorimeter for Gamma-ray Space Telescopes



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



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



# MC Codes available to our group to simulate coherent interactions of charged particles in oriented crystals

- In general purpose MC particle tracking codes, like Geant4, **matter is natively described as homogeneous, isotropic, amorphous.**
- **CRYSTAL**: code developed in Fortran by V. Tikhomirov. It is based on the Baier-Katkov quasi-classical method and can consider many effects, but each time must be manually adapted to the specific case...
- **CRYSTALRAD**: code developed in C++ by A. Sytov (it includes RADCHARM routine developed by L. Bandiera for radiation, also based on Baier-Katkov method).
- **Crystal support introduced in Geant4** by E. Bagli (former colleague) since Geant4 10.3. It allows the user to define a crystal from the unit cell → ab-initio approach, but includes only particle deflection, not radiation nor strong field effects...
- **Now**, we use **two different approaches** to simulate in **Geant4** respectively:
  - 1) **Particle deflection and radiation** → it makes use of a **Fast Simulation** model to stop the standard tracking inside selected volumes and run a code, **G4ChannelingFastSimModel** (included in Geant4 11.2), which is similar to CRYSTALRAD (A. Sytov).
  - 2) **Electromagnetic shower boost due to strong field effects** → through **bremsstrahlung and pair-production cross sections modification**, as a function of energy and angle w.r.t. desired axis, according to the results obtained through CRYSTAL code (which is based on the Baier-Katkov quasi-classical method). Mainly developed by V. Haurylavets.
- At the moment, we have **not yet implemented** a full simulation including **coherent pair-production** (not required for **positron source** simulation).

# 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 //.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....ooo00000ooo.....
82
83 G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
84 {
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

# How to use the Geant4 channeling model in your example?

## ● In the DetectorConstruction:

```
//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

```
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

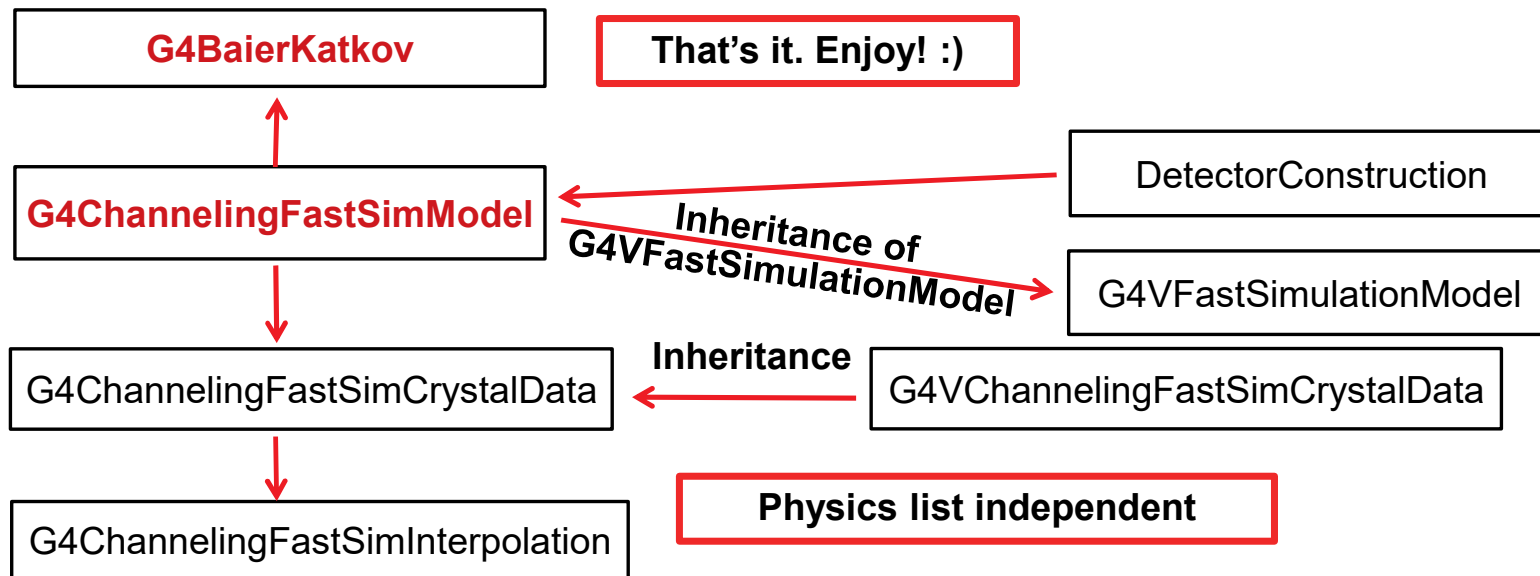
Radiation model  
activation

# How to use the Geant4 channeling model in your example?

- Add to main (or in a PhysicsList):

**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 );
```



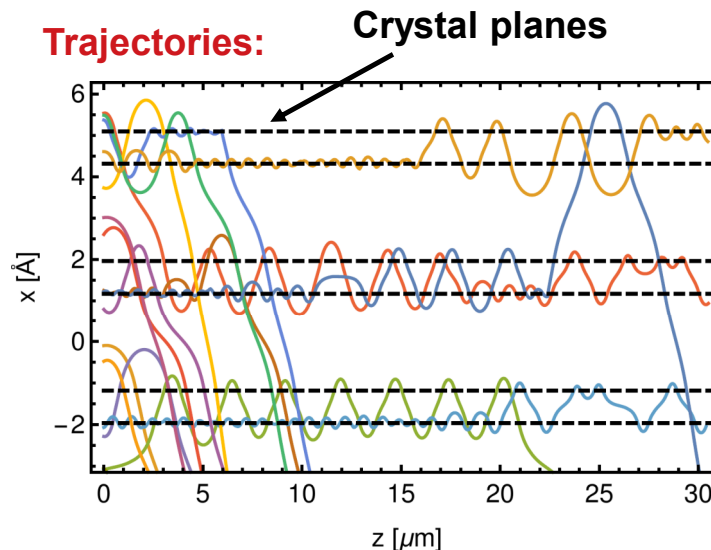


# Channeling simulation technique: **G4ChannelingFastSimModel**

- **Channeling** model using FastSim interface (trajectories): **READY** A. Sytov and G. Paternò  
@INFN Ferrara
- **Radiation** model (Baier-Katkov method) —————> **TESTING NOW**
- **Radiation** and **positron source Geant4** examples —————> **FOR SOME MATERIALS**



This model, together with **multiple and single Coulomb scattering** on nuclei and electrons and standard or pre-calculated (through BK) **pair-production CS**, allows us to simulate the **Radiator Crystal** for positron sources



channeling\*



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

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)

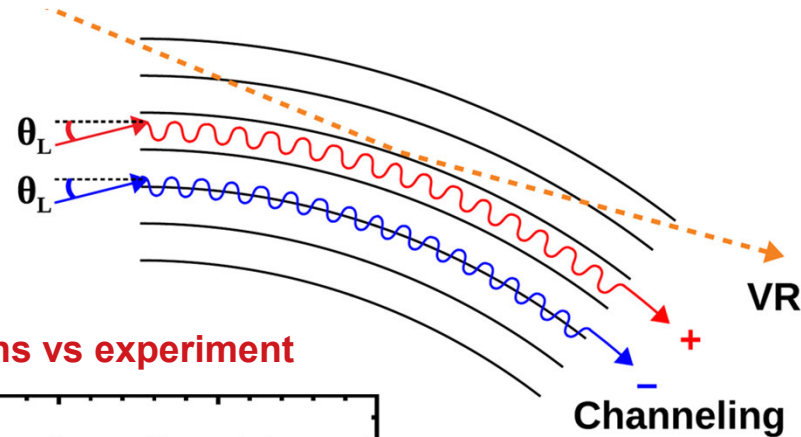
\*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

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



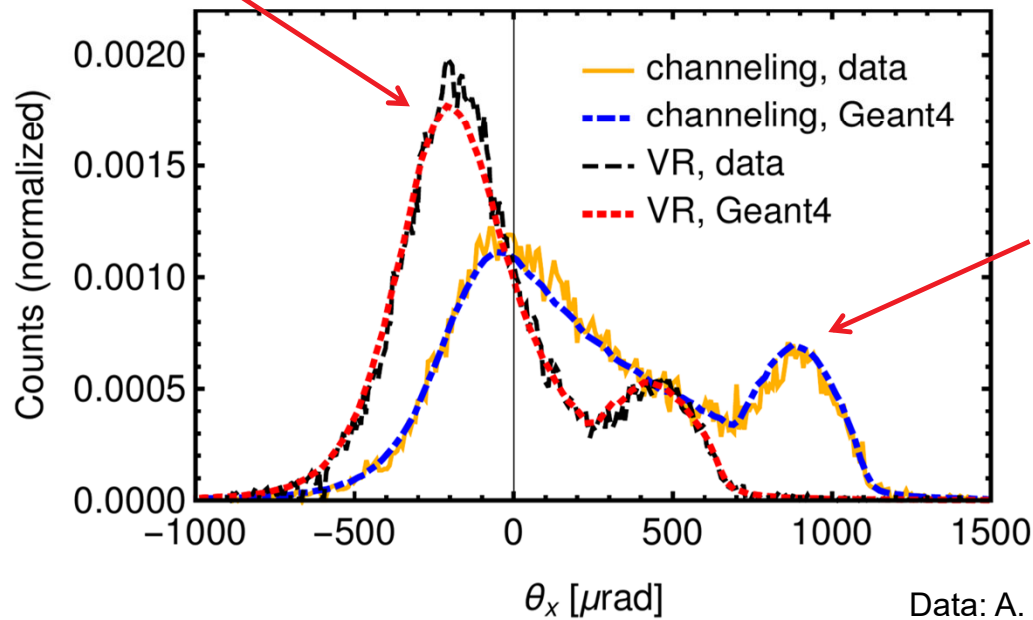
855 MeV  
electrons

15  $\mu\text{m}$  thick bent  
crystal



volume reflection (VR)

Geant4 simulations vs experiment



channeling

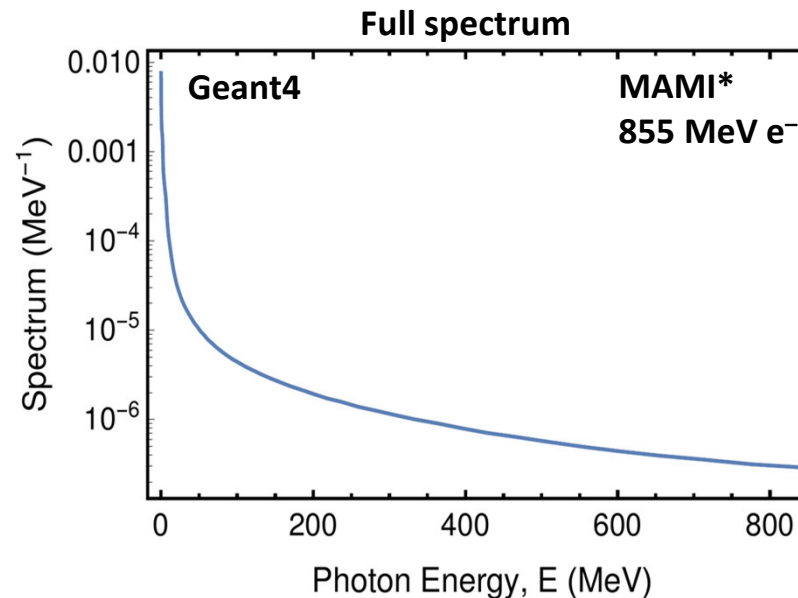
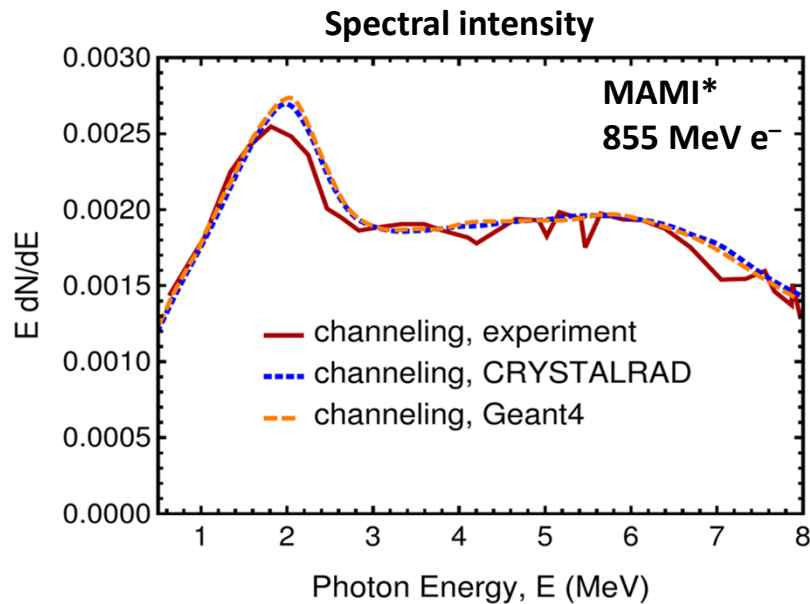
Data: A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

# 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**

## Geant4 simulations vs experiment and CRYSTALRAD simulations



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

# Current **Geant4** applications useful to simulate coherent interactions of charged particles in oriented crystals

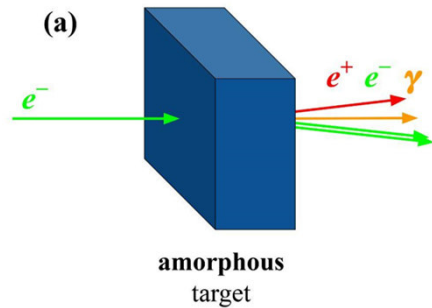
- **FastSimChannelingRad**: it allows us to test *G4ChannelingFastSimModel* for different crystalline materials and orientations.
- **OCalo4Sat**: it can be used to simulate electromagnetic calorimeters composed of oriented crystals. It can take advantage both of *G4ChannelingFastSimModel* model and EM shower boost based on cross-section modification.
- **PositronSource**: it can be used for the optimization of a Positron Source based on oriented crystals. It is based on the *G4ChannelingFastSimModel* model.
- **TestBeamOC**: it is conceived to simulate the experiments with oriented crystals we carry out at different facilities. It is **currently under development**, but specific versions implemented by M. Soldani and P. Monti-Guarnieri and based on previous coherent models are available.

*These applications are continuously developed by me within the framework of various projects, e.g. **Geant4infn**.*

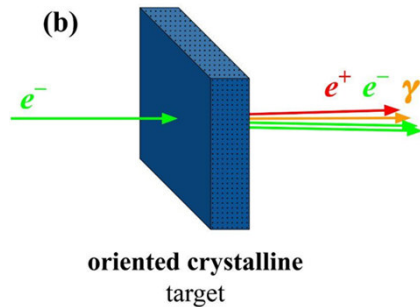
# Positron source for future lepton colliders

## UNPOLARIZED POSITRON SOURCES

### 1. Conventional

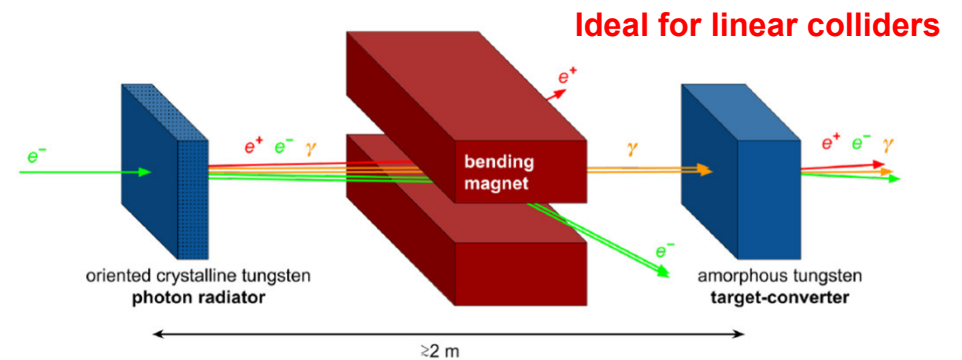
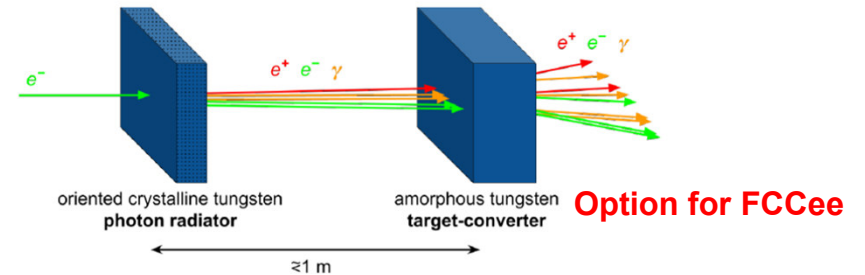


### 2. e+ from channeling radiation



Tests performed at CERN (WA 103) and at KEK

### 3. Hybrid crystal-based positron source

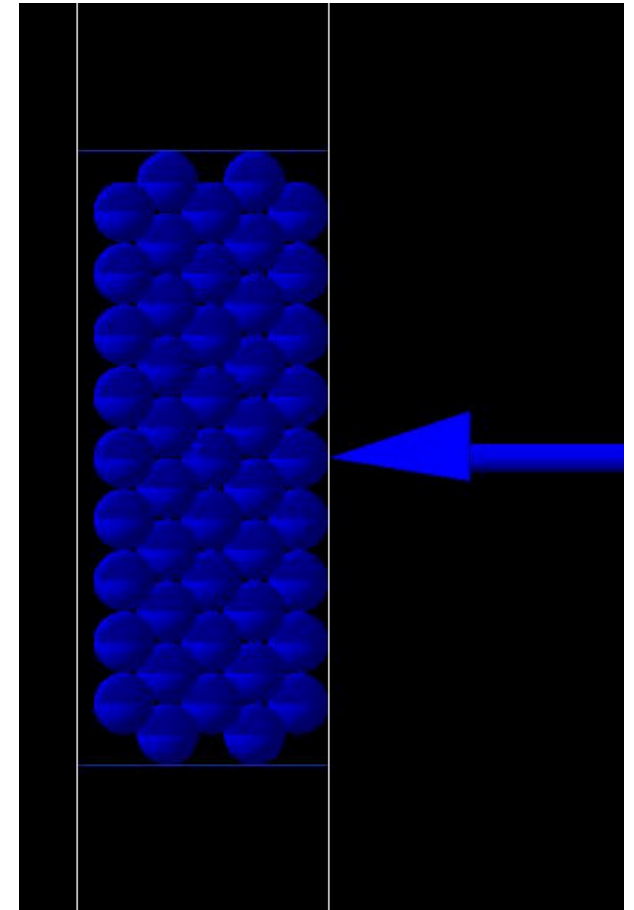
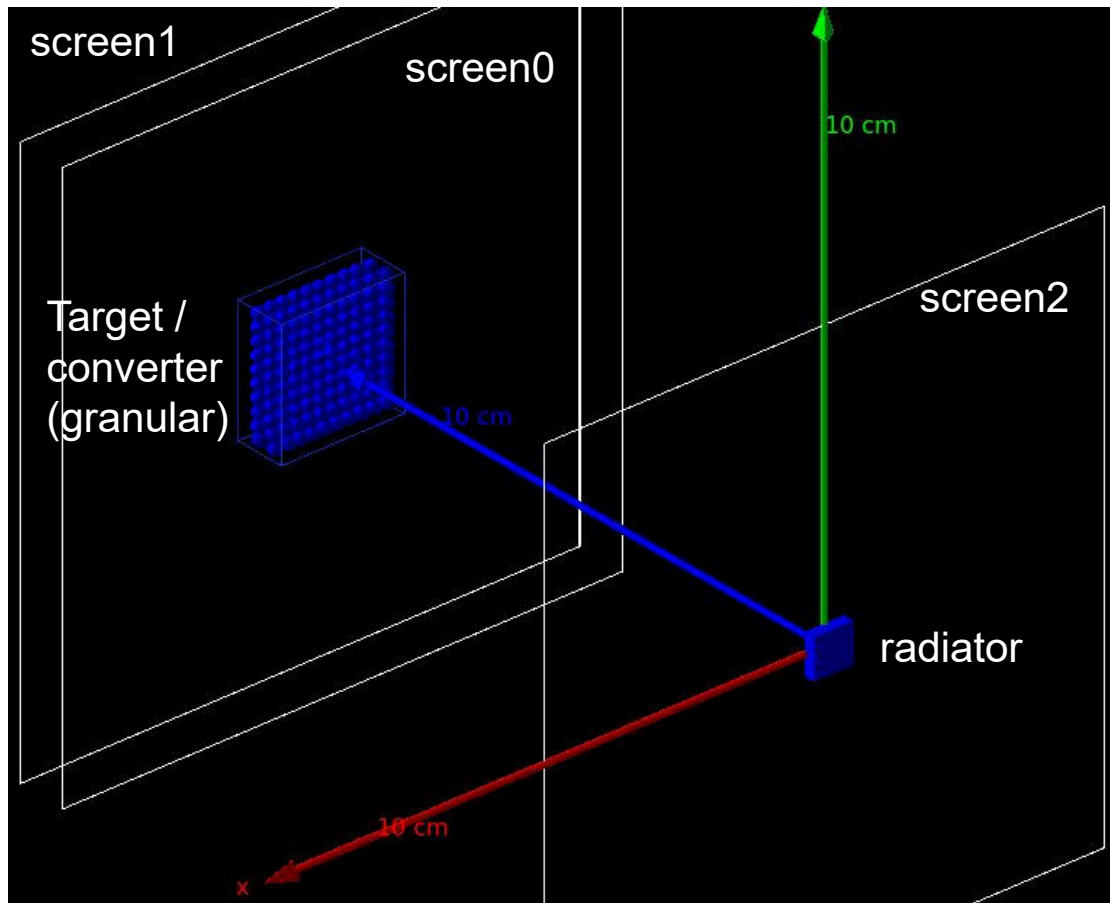


Idea of R. Chehab, V. Strakhovenko and A. Variola, NIM B 266 (2008) 3868

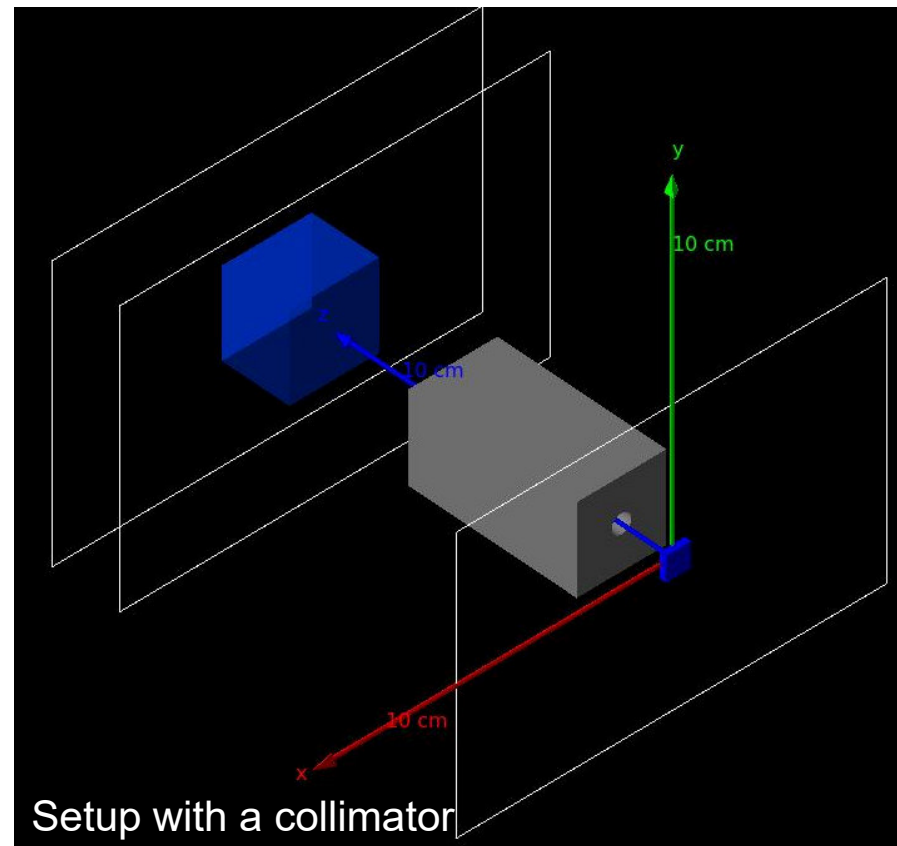
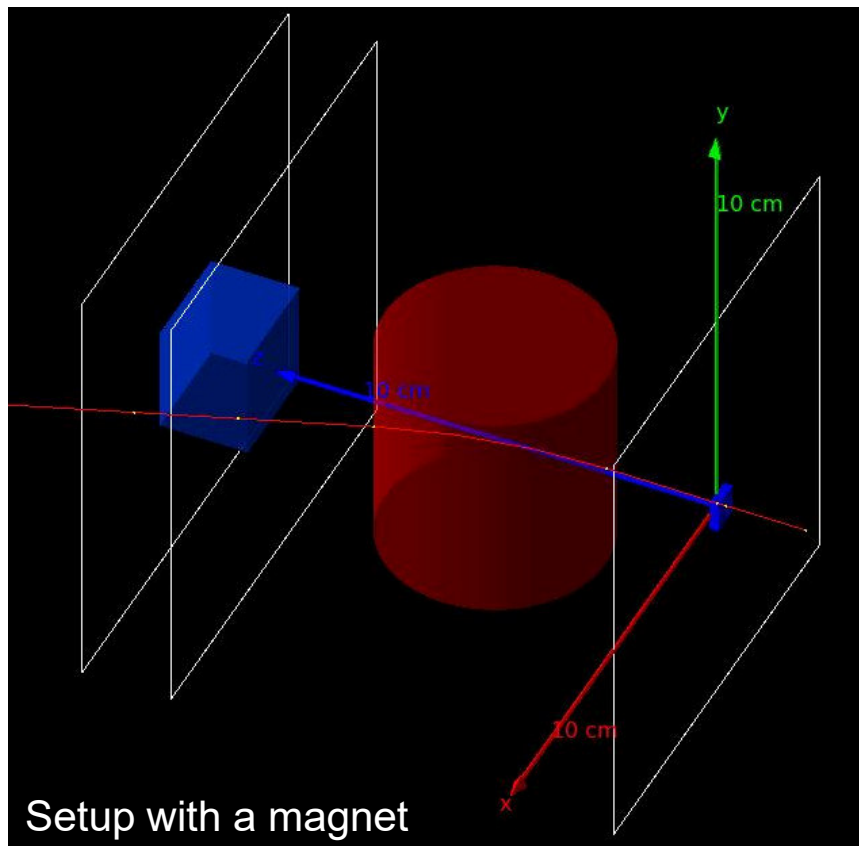
# PositronSource Geant4 application

- It allow us to simulate a crystal-based Positron Source, according to the previous schemes, namely **conventional, oriented-crystal and hybrid positron sources**.
- The code relies on ***G4ChannelingFastSimModel*** to simulate coherent effects in crystals. Alternatively, the phase-space of particles obtained through CRYSTAL code can be imported and tracked into the considered setup.
- Apart from converter (which can be granular) and radiator crystals, a region with a **magnetic field** or a **collimator** can be included in the setup.
- The **scoring** is made through 1-3 virtual scoring screens to store a **root ntuple**: (screenID,particle,x,y,px,py,pz,t,eventID) at the exit of the radiator and at entrance and exit of the converter. Also, the **energy deposited in the crystals per event** is recorded, as well as the **energy distribution (voxelized)** in the converter (or the radiator) in a text file.
- The application is fully compatible with **multi-threading**.
- A set of **custom commands** have been created; thus, the user does not need to re-compile the application to change a parameter. The entire setup can be controlled -> very useful for a systematic study.
- The code, as well as scripts and result files, can be found in this **Drive shared folder**:  
[https://drive.google.com/drive/folders/11GbITtv1djkIzjISzMkdf7BgF415n6Bs?usp=drive\\_link](https://drive.google.com/drive/folders/11GbITtv1djkIzjISzMkdf7BgF415n6Bs?usp=drive_link)

# PositronSource Geant4 application



# PositronSource Geant4 application





# PositronSource Geant4 application

```
#Positron Source type
#/det/isHybridSource false          #default true

#Radiator Crystal settings
/crystal/setCrystalMaterial W       #PWO, BGO, C, W, Ge, Si (default)
/crystal/setCrystalSize 7. 7. 2. mm
/crystal/setCrystalLattice <111>   #planes (e.g. (111)) or axes (e.g. <111>)
#/det/setRadiator true              #default is false (if !isHybridSource -> automatically true)

#Converter Crystal settings
/det/setRadiatorConverterSepDistance 50. cm
/det/setConverterSize 199.75 199.75 11.6 mm #th=17.6mm->conventional, th=11.6mm->hybrid
#/det/setGranularConverter true      #default is false
#/det/setSphereRadius 1.1 mm

#other geometry settings
#/det/setMagneticField true          #default is false
#/det/setMagneticFieldValue 5. tesla
#/det/setMagneticFieldRegionLength 20. cm

#/det/setCollimator true             #default is false
#/det/setCollimatorAperture 5.5 mm
#/det/setCollimatorThickness 50. cm
#/det/setCollimatorSide 2.5 m
#/det/setRadiatorCollimatorSepDistance 5. cm

#/crystal/setVirtualDetectorSize 40. 40. 0.001 cm

#Voxelization settings
/det/setVoxelization true            #activate the voxelization of the Converter Crystal (default false)
/det/setColumns 401                  #799
/det/setRows 401
/det/setSlices 24                    #36 for th=17.6mm, 24 for th=11.6mm
#/det/setAbsorberDxVoxel 1. mm
#/det/setAbsorberDyVoxel 1. mm
/det/setAbsorberDzVoxel 0.5 mm

/run/initialize
```

run.mac

# PositronSource Geant4 application

```
/run/initialize

/control/verbose 0
/run/verbose 1 #to see the Couples CutsVsRegion
/tracking/verbose 0
#/run/dumpCouples

/run/setfilenamesave output/output_6GeV_W2p0mm_readPS_D50cm.root

/gun/ReadFromFile true #default false
/gun/SetFileName input/W2.0mm_6GeV_all.dat #put these lines after /run/initialize

#beam
/gps/particle e-
#coordinate distribution
/gps/pos/centre 0. 0. -5. cm
/gps/pos/type Beam
/gps/pos/sigma_x 0.5 mm
/gps/pos/sigma_y 0.5 mm
#angular distribution
/gps/ang/type beam2d
/gps/ang/rot1 1 0 0
/gps/ang/rot2 0 -1 0
/gps/ang/sigma_x 100.E-6 rad
/gps/ang/sigma_y 100.E-6 rad
#energy distribution
/gps/ene/mono 6. GeV

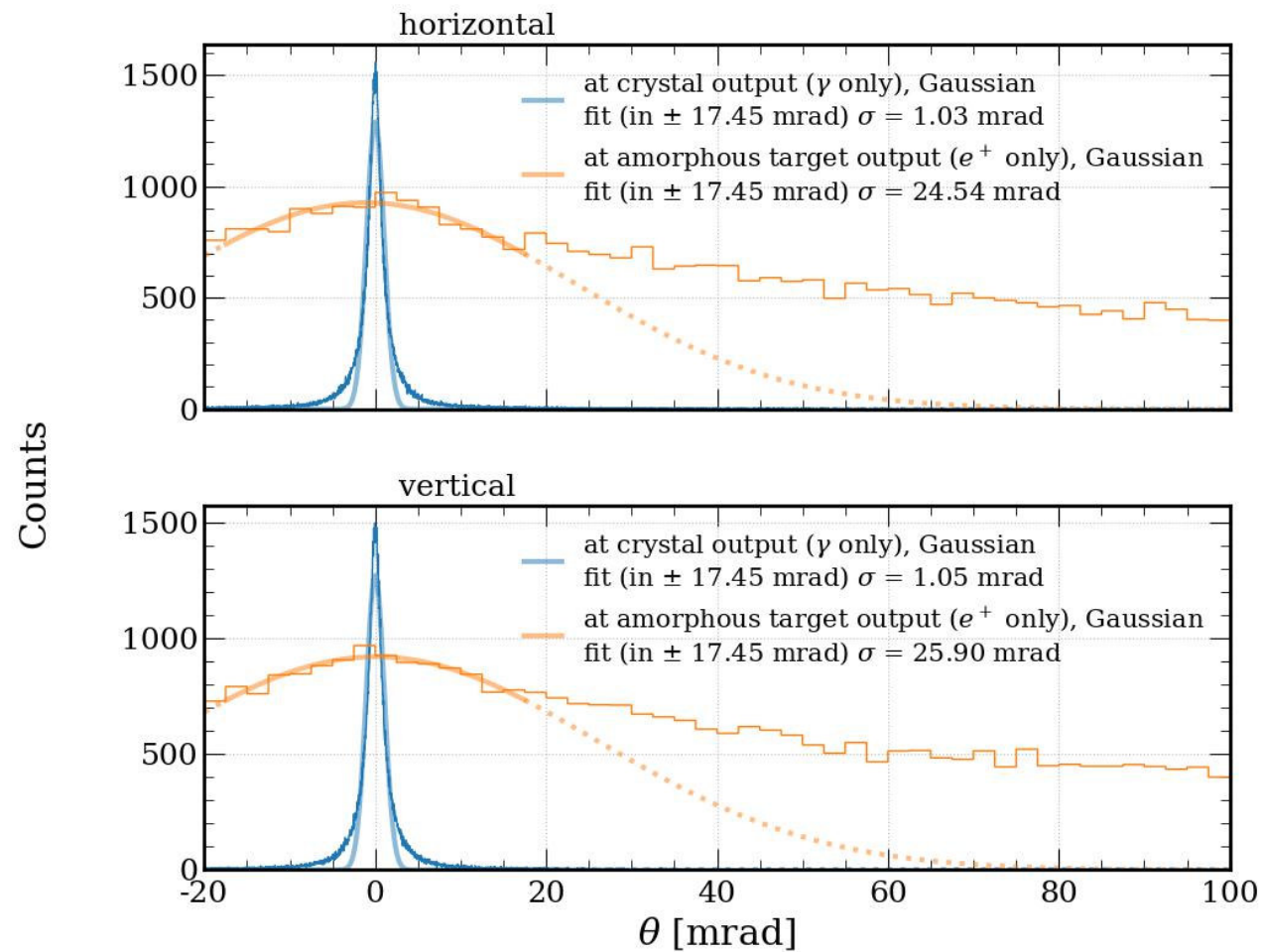
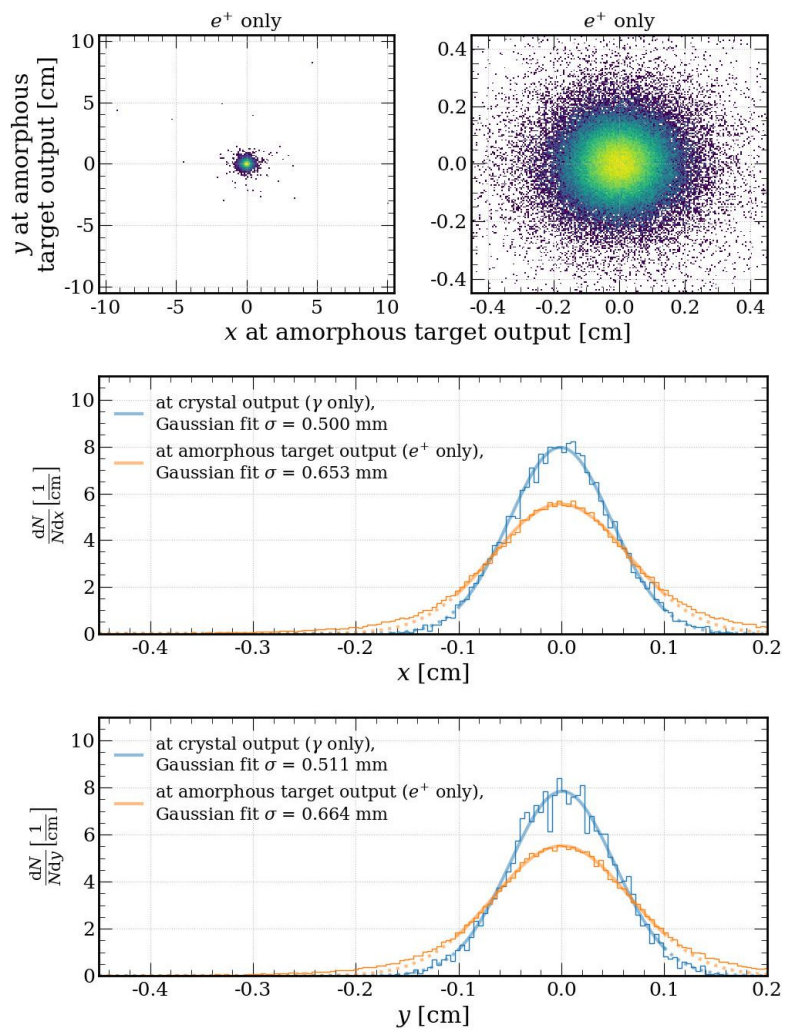
#/score/create/boxMesh boxMesh1
#/score/mesh/boxSize 99.875 99.875 5.8 mm #semi-quantities (z=8.8 for th=17.6mm, 5.8 for th=11.6mm)
#/score/mesh/nBin 401 401 24 #799 799 36
#/score/mesh/translate/xyz 0. 0. 505.83 mm #[505.83 if D=500 or 5.82 if D=0] CHECK ALWAYS! <-----
#/score/quantity/energyDeposit Edep #[MeV];
#/score/close
#/score/list

#statistics
/run/printProgress 100
/run/beamOn 236741 #10000 #236741 #353796

#/score/dumpQuantityToFile boxMesh1 Edep output/Edep 6GeV W2.0mm readPS D50cm.txt
```

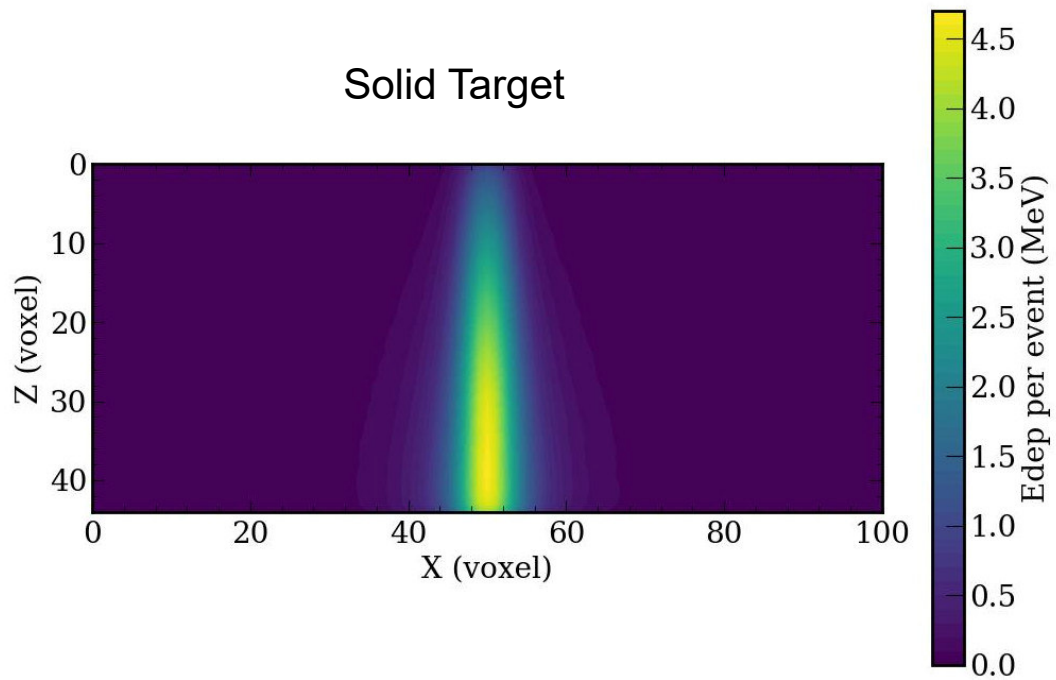
run.mac

# PositronSource Geant4 application

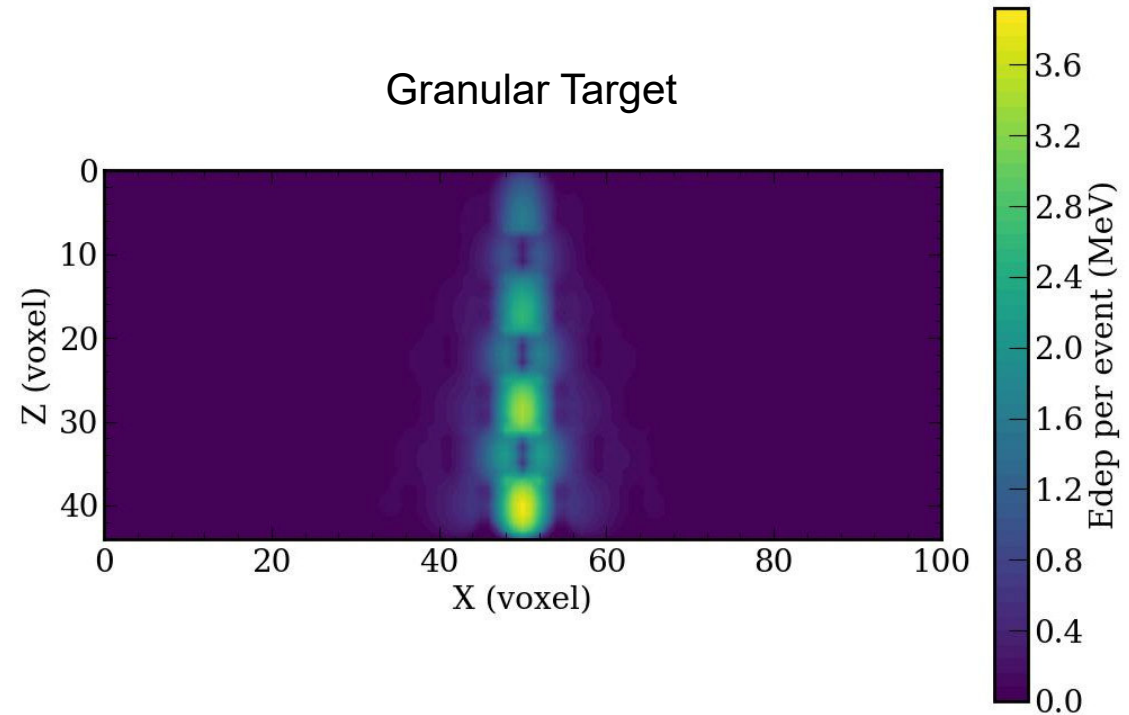


# PositronSource Geant4 application

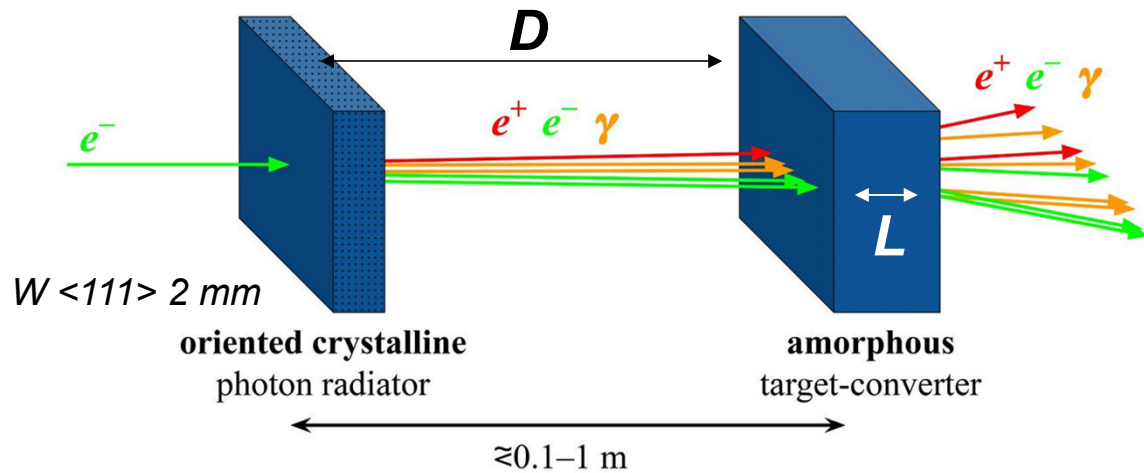
Solid Target



Granular Target



# Hybrid source optimization for FCC-ee

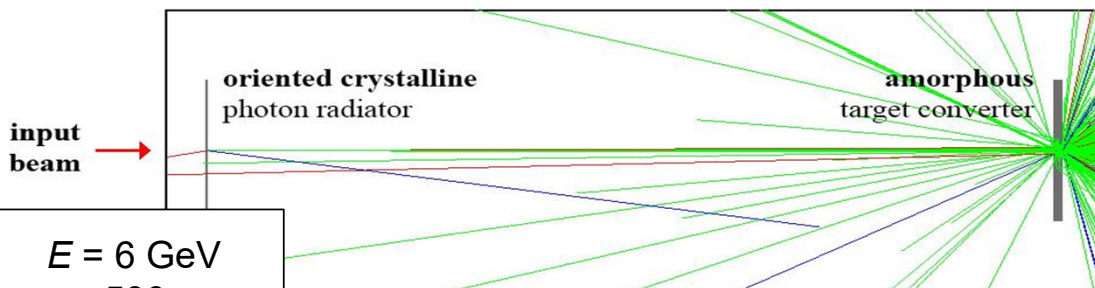


energy deposit and PEDD in amorphous converter can be reduced by tuning  $L$  (while keeping the radiator thickness fixed to maximise EM enhancement) and  $D$

**Geant4** simulation of the downstream stage...

(*upstream stage already optimised with dedicated code and experimental data* → *dedicated input files*)

— photons — electrons — positrons



$E = 6 \text{ GeV}$   
 $\sigma = 500 \mu\text{m}$   
 $\sigma' = 100 \mu\text{rad}$

L. Bandiera *et al.*, **EPJC** 82, 699 (2022)

Collaboration with IJCLab (leader I. Chaikovska)

**The starting point:** results reported in **M. Soldani et al, NIMA, 2024,**  
<https://doi.org/10.1016/j.nima.2023.168828>

Scheme	conv.	hybrid						
$L_{\text{crys}}$ [mm]	–				2			
$D$ [m]	–	0.6		1			2	
$L$ [mm]	17.6				11.6			
( $a = 5.5$ mm) Collimator?	no	no	no	yes	no	no	yes	no
Magnet?	no	no	no	no	yes	no	no	yes
$E_{\text{dep}}$ [GeV/ $e^-$ ]	1.46	1.34	1.32	1.13	1.32	1.27	1.11	1.27
PEDD [MeV/( $\text{mm}^3 \cdot e^-$ )]	38.3	12.8	8.4	8.2	8.4	4.1	3.8	3.9
Out. $e^+/e^-$	13.7	15.1	15.1	13.6	15	14.9	13.7	14.9
Out. $e^+$ beam size [mm]	0.7	1	1.2	1.2	1.2	1.5	1.5	1.5
Out. $e^+$ beam div. [mrad]	25.9	27.4	26.8	27.7	28.9	29.2	25.6	27.1
Out. $e^+$ mean energy [MeV]	48.7	46.2	45.6	47.4	45.9	46.1	47.7	46.3
Out. $n/e^-$	0.37	0.31	0.31	0.27	0.29	0.29	0.26	0.3
Out. $\gamma/e^-$	299	310	308	270	307	301	268	301

conventional  
(amorphous)  
collimator  
magnet

We need to  
improve the  
capture  
efficiency of  
the downstream  
stage (not  
reported here)

# Summarizing...

- We have different options to simulate coherent interactions of charged particles in oriented crystals.
- The simulation environment has now been fully developed and can be used for more sophisticated studies (e.g., capture simulations), in order to arrive to the conceptual design for the hybrid scheme. In parallel, other crystals can be simulated and checked. Eventually, the performance will be compared to the conventional scheme.