Istituto Nazionale di Fisica Nucleare

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Trillion

High performance Geant4 simulations of electromagnetic processes in oriented crystals

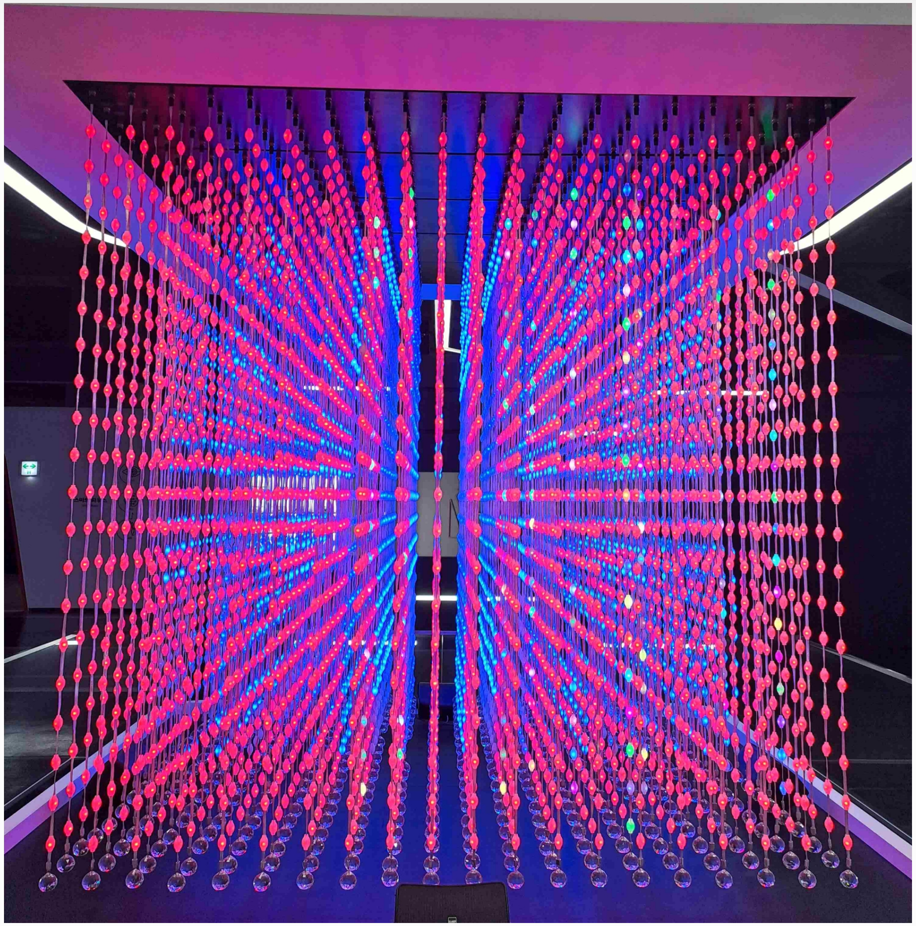
Dr. Alexei Sytov, Prof. Kihyeon Cho, Dr. Laura Bandiera

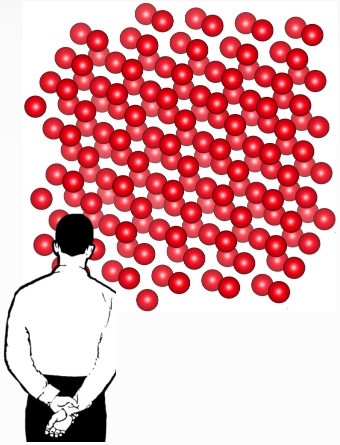
sytov@fe.infn.it

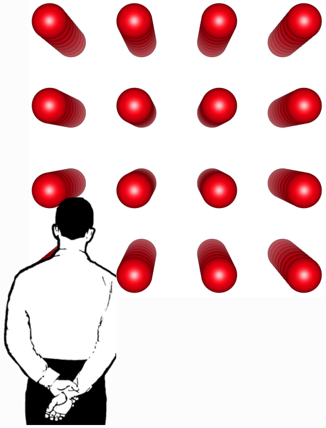
International Symposium on Grids & Clouds (ISGC) 2023

Taipei, Academia Sinica, 24/03/23

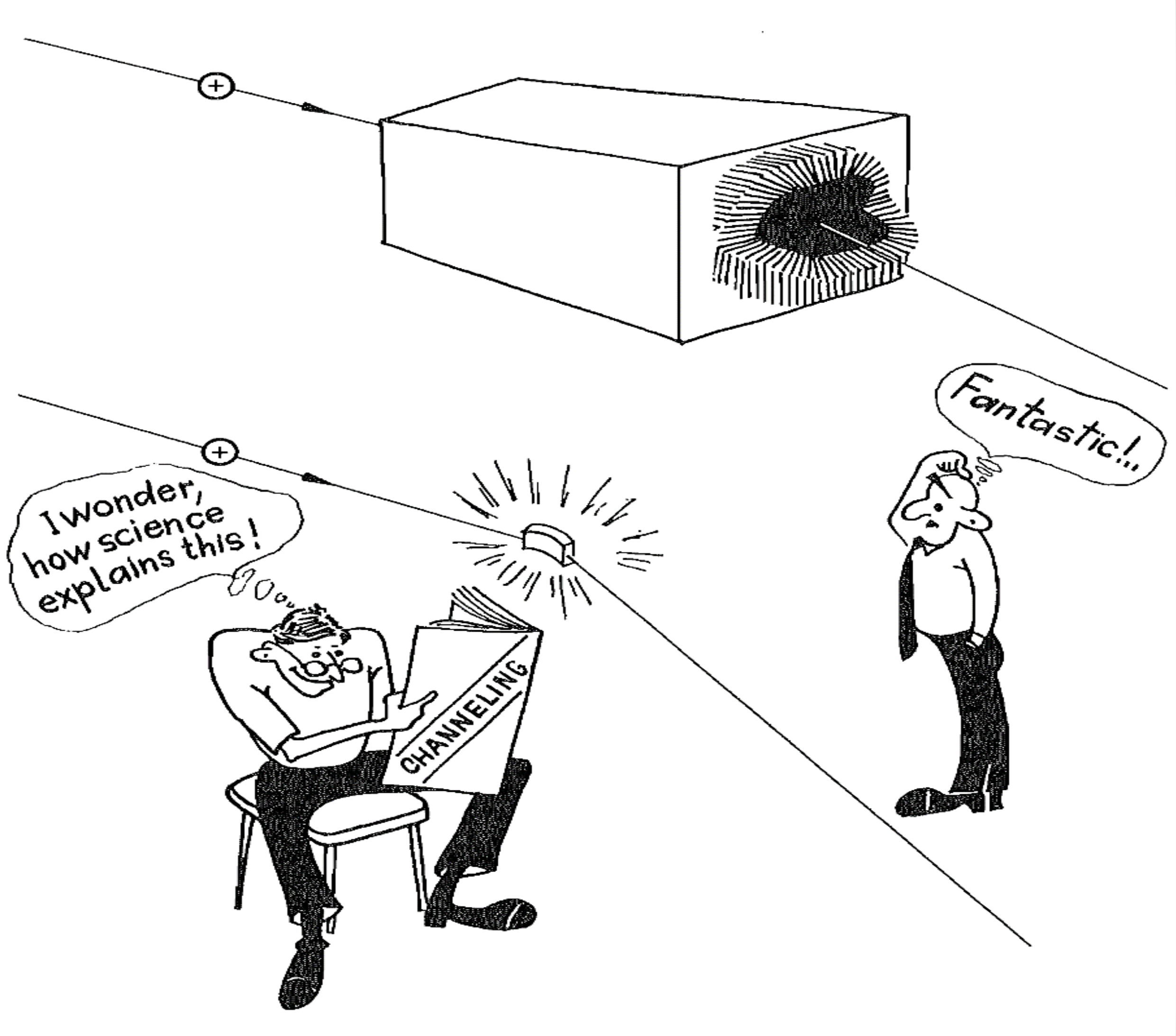
How a crystal lattice look like
(from National Science Museum, Daejeon, Korea)



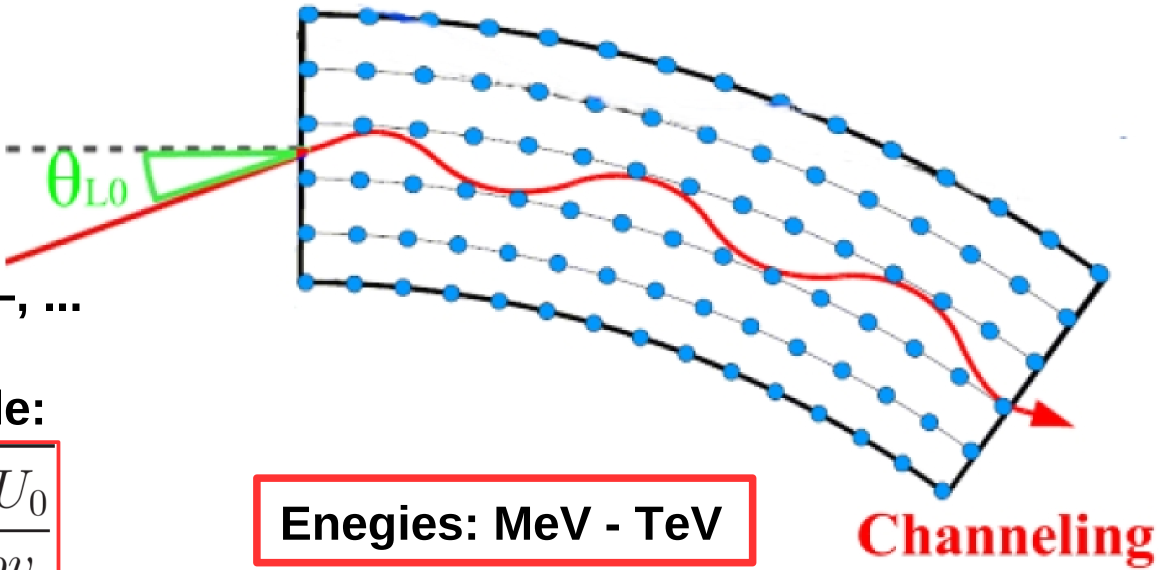




The world of the channeling effect



Channeling effect* of charged particles



proton, e+, e–, ...

Lindhard angle:

$$\theta < \theta_L = \sqrt{\frac{2U_0}{pv}}$$

Enegies: MeV - TeV

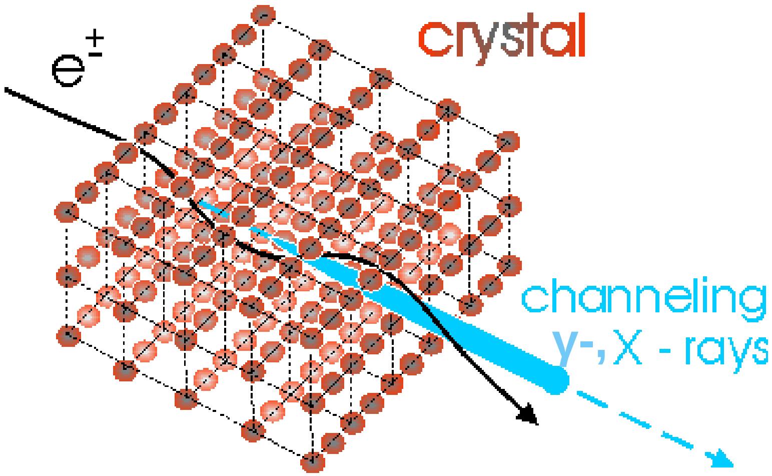
Channeling* **is the effect of the penetration of charged particles through a monocrystal quasi parallel to its atomic axes or planes.**

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

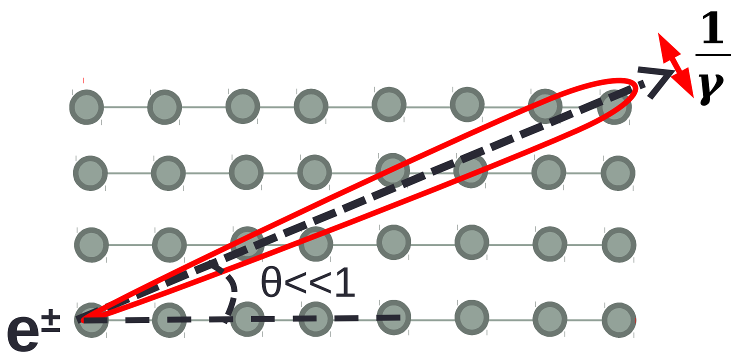
*J. Stark, Zs. Phys. 13, 973–977 (1912)
J. A. Davies, J. Friesen, J. D. McIntyre, Can J. Chem. 38, 1526–1534 (1960)
M. T. Robinson, O. S. Oen, Appl. Phys. Lett. 2, 30–32 (1963)
J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)

Coherent effects in a crystal

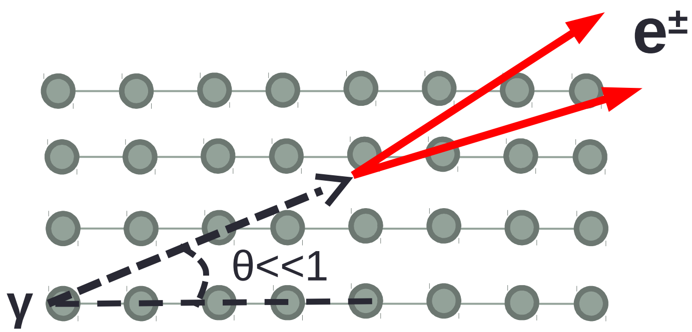
Channeling radiation*



Coherent bremsstrahlung**



Coherent pair production***



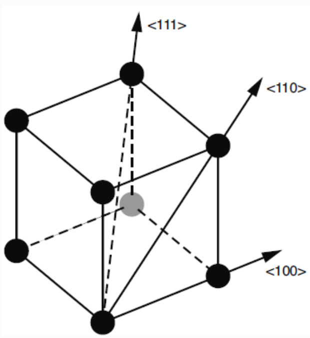
Coherent effects preserve **up to few mrad** of particle direction vs the crystal axis

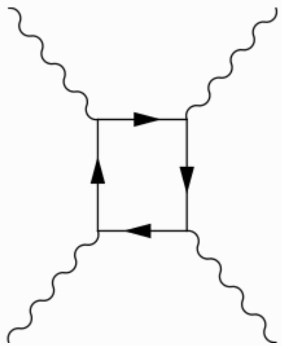
***M.A. Kumakhov, Phys. Lett. A 57(1), 17–18 (1976)**
****B. Ferretti, Nuovo Cimento 7, 118 (1950).**
****M. Ter-Mikaelian, Sov. Phys. JETP 25, 296 (1953).**
***** H. Überall, Phys. Rev. 103, 1055 (1956).**

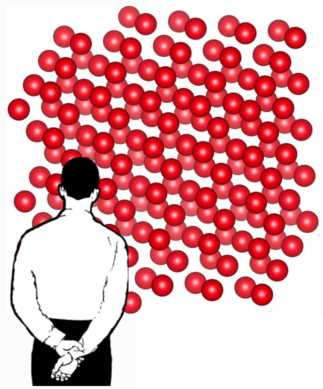
Electromagnetic shower acceleration

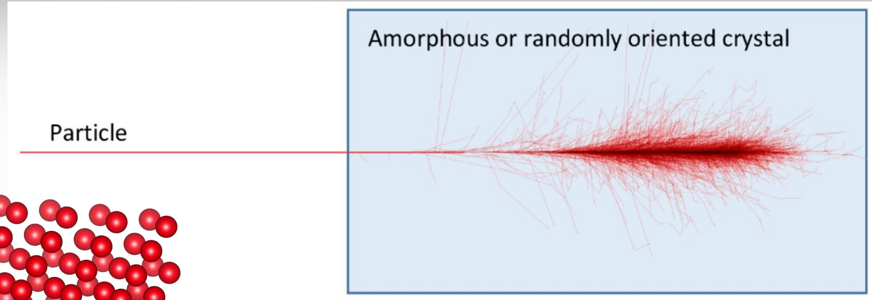
Axial field 10^{11} V/cm

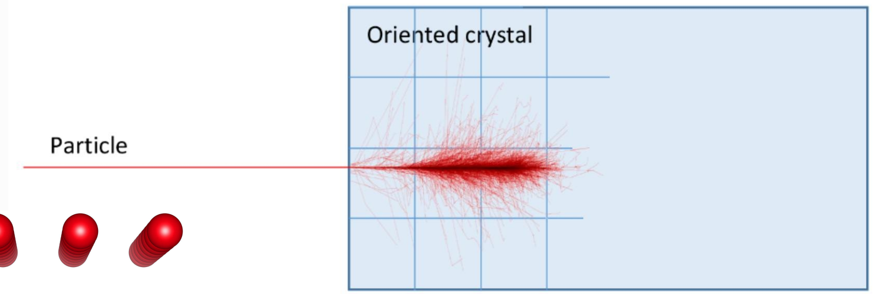
Approaching the **Schwinger limit** starting from few **GeV** for **e+/e-**

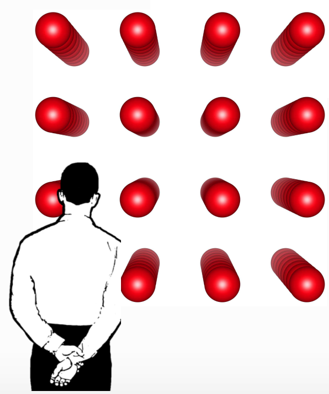








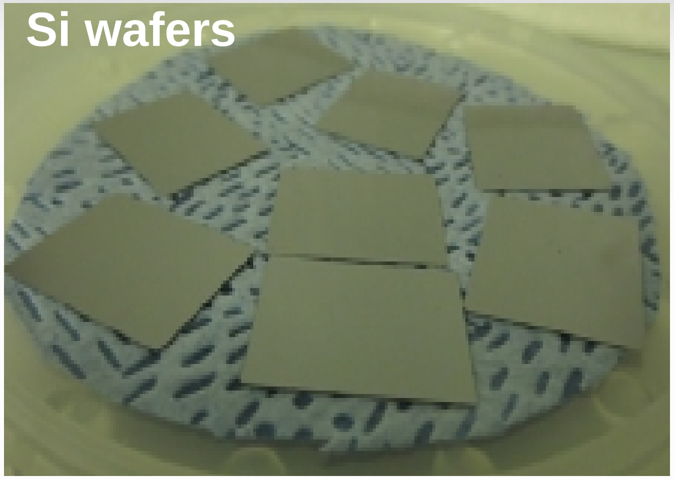


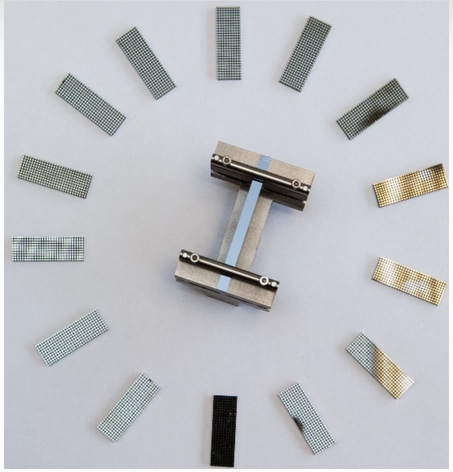


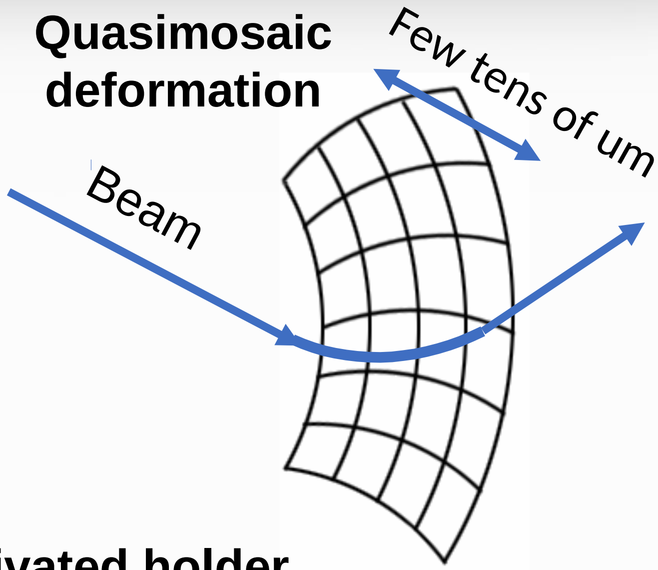
The **radiation** intensity and the **pair production** cross-section **drastically increase** in **oriented crystals!**

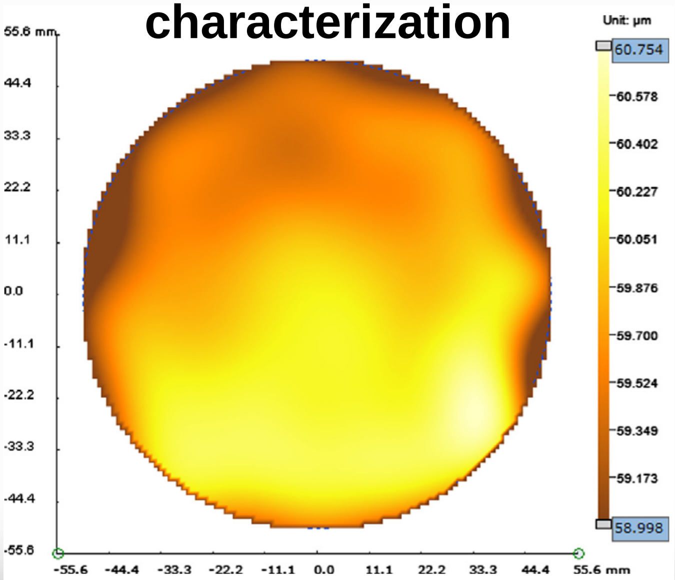
Shower development in the field of axes is **accelerated**. The radiation length is considerably reduced*.

Manufacturing and characterization of bent silicon crystals @INFN Ferrara

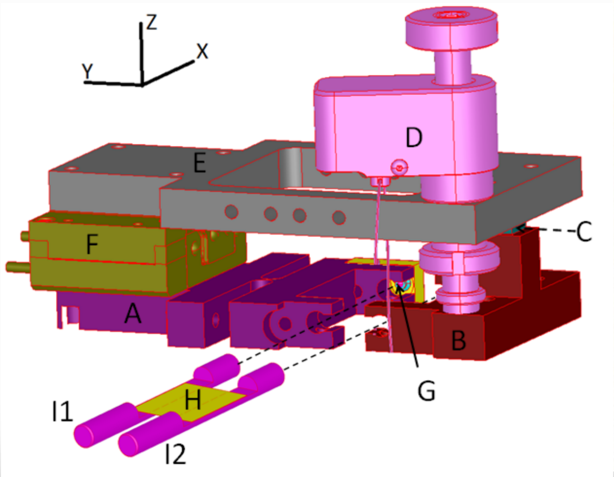


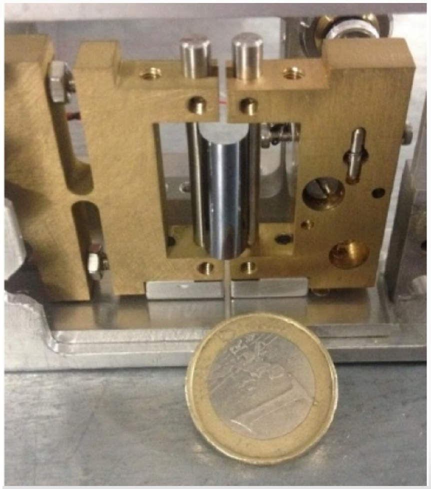






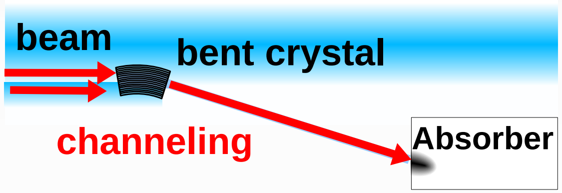
Piezo-activated holder



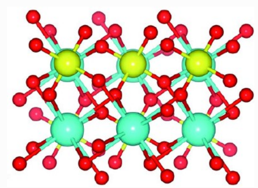


Applications*

Crystal-based collimation or beam extraction from an accelerator

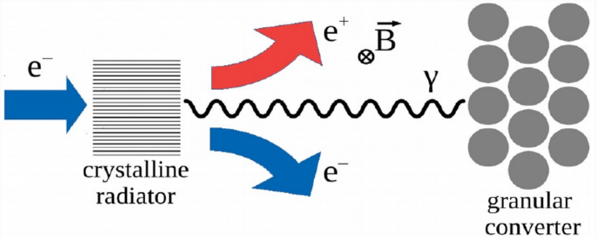


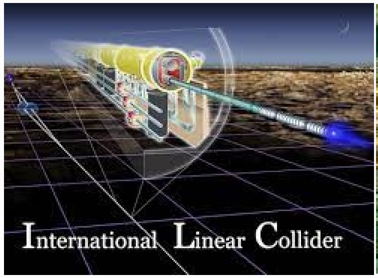
Ultrashort crystalline calorimeter

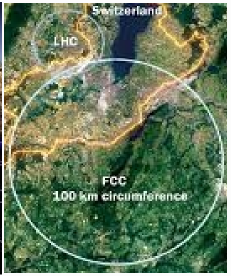


Gamma-ray Space Telescope

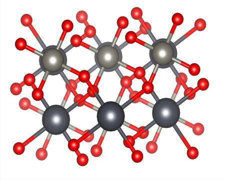
Positron source for future e+/e- and muon colliders



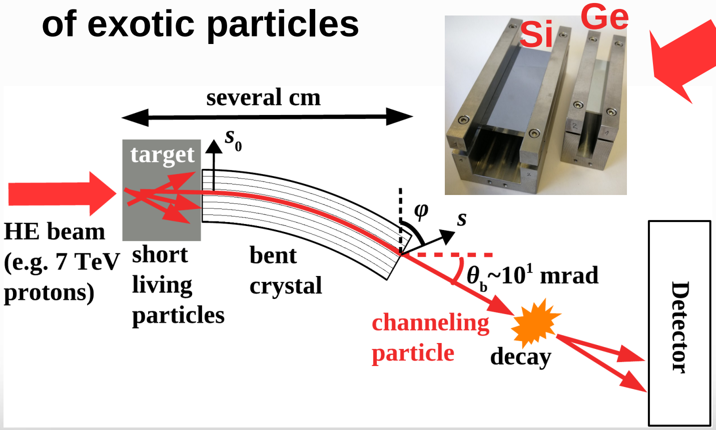




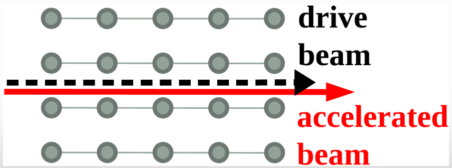
Oriented crystals



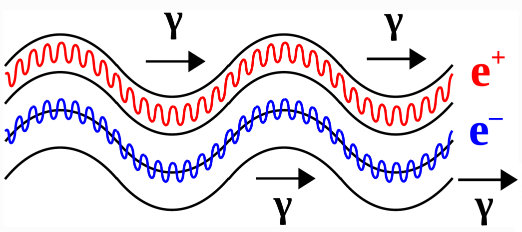
Measurement of dipole magnetic and electric moments of exotic particles

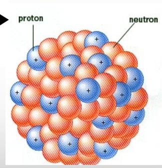


Plasma acceleration



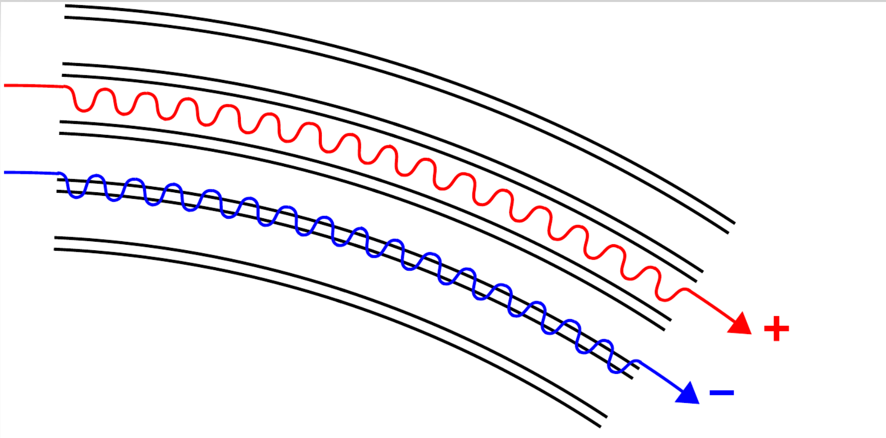
X and γ-ray source for nuclear and medical physics





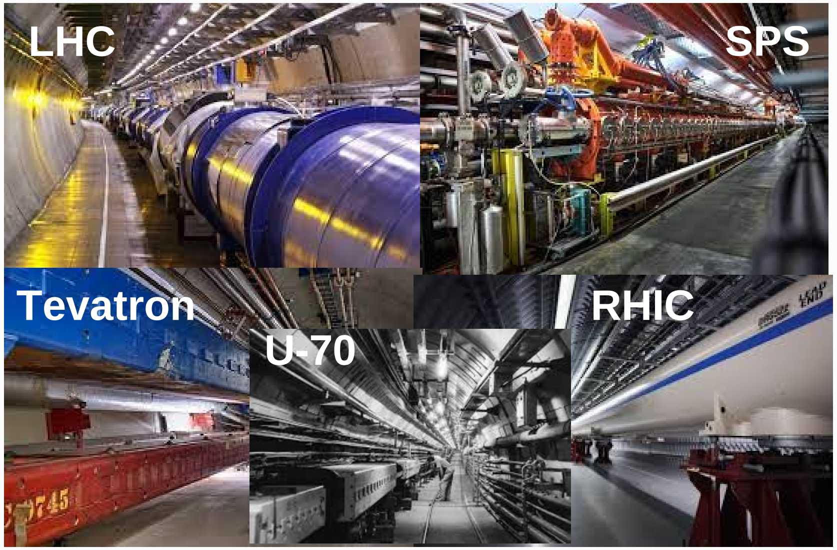
*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

Crystal-based extraction

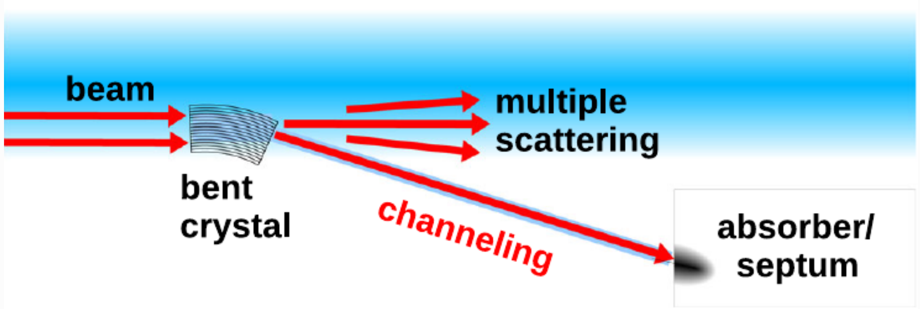


Planar channeling*:
Charge particle penetration through a monocrystal along its atomic planes

Crystal-based collimation and **extraction have been used at hadron machines**



Crystal-based extraction/collimation



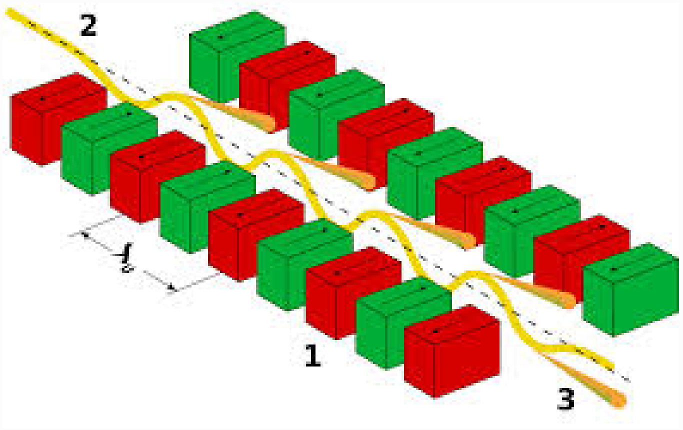
Crystal-based extraction/collimation: applied only for hadrons, not yet for e-

Interesting for tens of electron synchrotrons

*J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)
E.N. Tsyganov, Fermilab TM-682 (1976)
A. Sytov et al. Eur. Phys. J. C 82, 197 (2022)

Channeling radiation in a bent crystal: Crystalline undulator

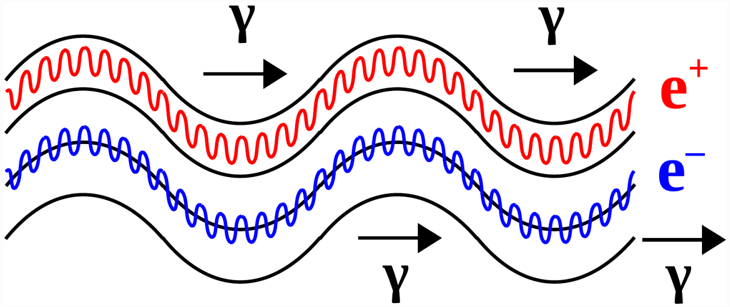
Classical scheme: magnetic undulator in a free electron laser soft X-rays $\lambda_u \sim$ cm



Advantage:

- Intense X- and gamma-rays produced in a crystal, in a compact piece of material

Innovative scheme: Crystalline undulator*-> Hard X-rays and gamma rays $\lambda_u <$ mm



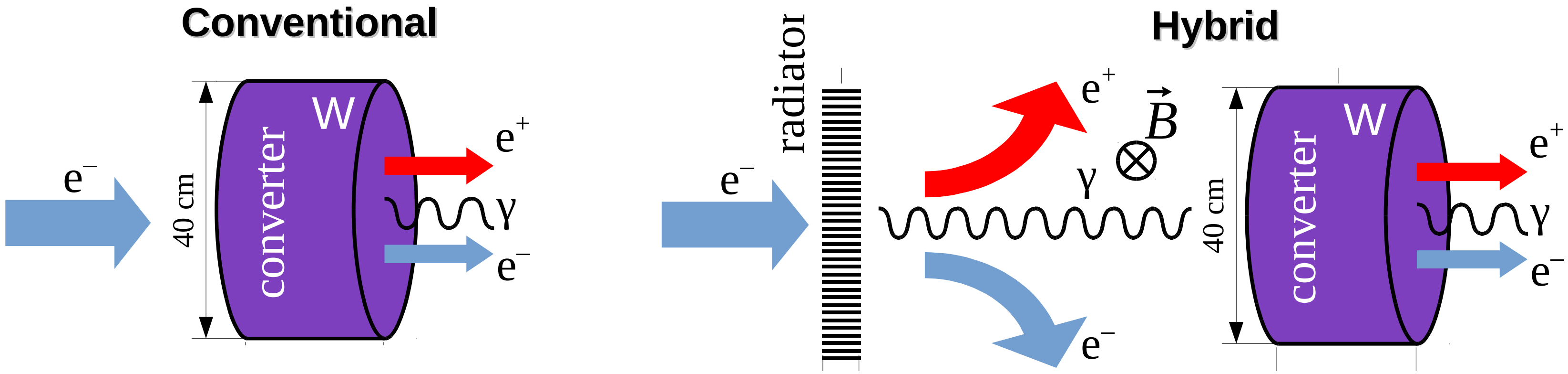
Crystalline X and gamma-ray source **can be applied** in:

- **Nuclear physics**
- **Medical physics**

EU project MSCA RISE N-LIGHT G. A. 872196
Coordinator MBN RESEARCH CENTER (Germany)

R. Camattari et al., Phys. Rev. Acc. and Beams 22, 044701 (2019)

Crystal-based hybrid positron source*



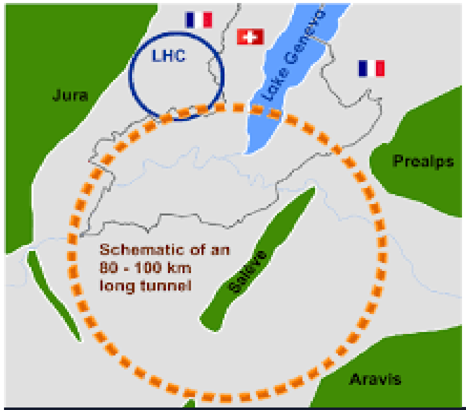
Coherent effects in a crystal **accelerate electromagnetic shower** development

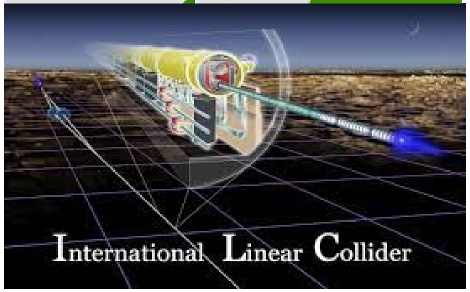
Advantages of the hybrid positron source:

- **Higher** positron yield
- Considerably lower peak deposited energy inside the target => **higher beam intensities**, **longer target lifetime**

Hybrid positron source can be applied at:

- **FCC-ee**
- **ILC**
- **Muon collider**



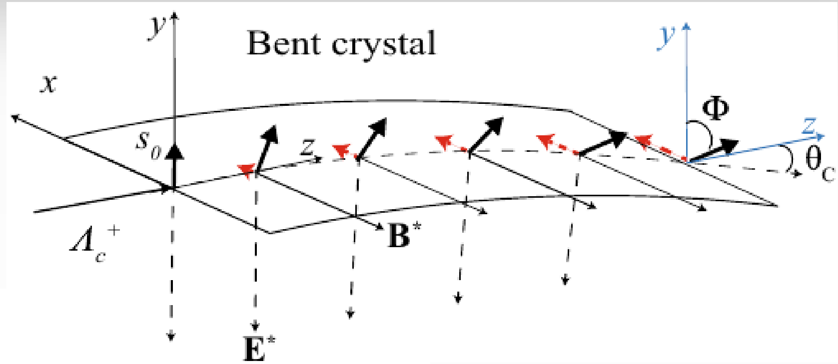


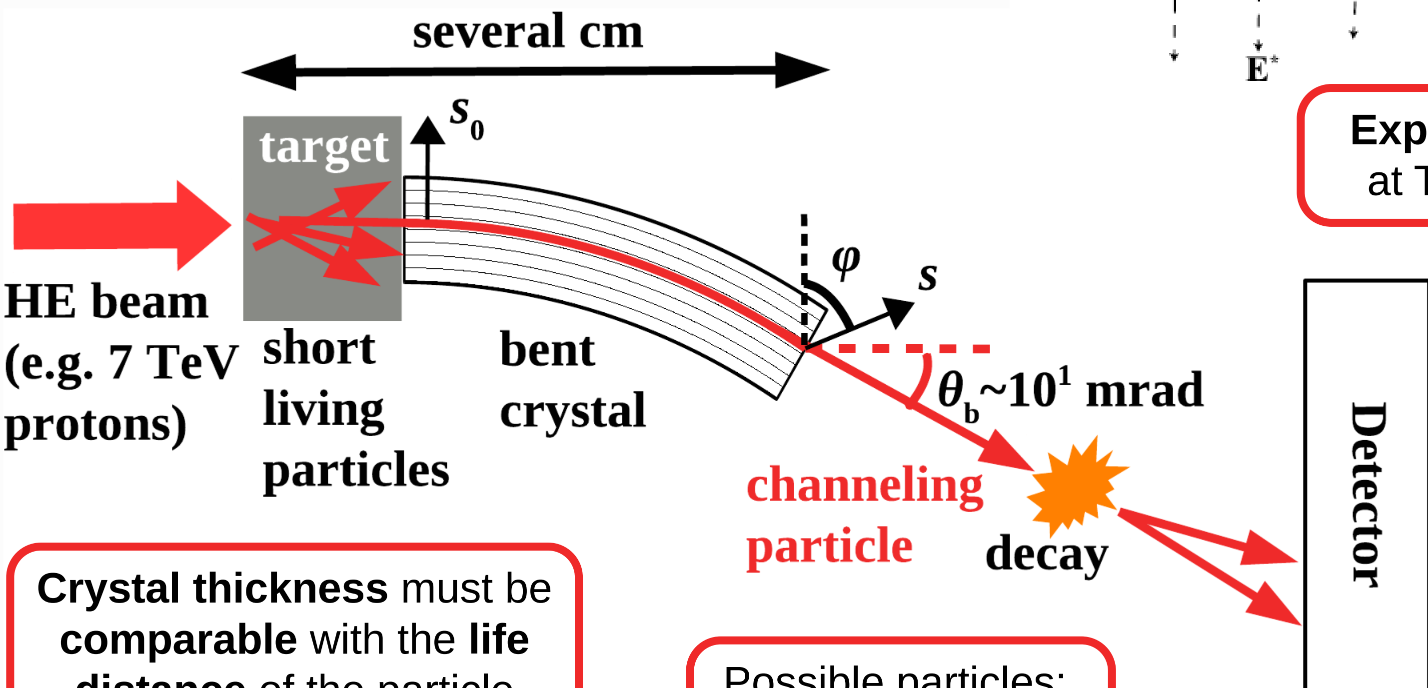
Simulation model can be also applied for **ultrashort crystalline calorimeter**

Search of MDM&EDM of short living particles using the effect of spin rotation in oriented crystals*

What we want:

- To measure **MDM** and **EDM** of exotic baryons





Experimental proof at Tevatron for Σ^+**

Crystal thickness must be **comparable** with the **life distance** of the particle

Possible particles: Λ_c^+, Ξ_c^+, ..., τ

* V. G. Baryshevskii, Pis'ma Zh. Tekh. Fiz. 5, 182 (1979)

**D. Chen et al. (E761 Collaboration) Phys. Rev. Lett. 69, 23 (1992)

Plasma wake-field acceleration in oriented crystals*

$$E[\mathrm{GV/m}] = m_e \omega_p c/e \approx 100\sqrt{n_0[10^{18}\mathrm{cm}^{-3}]}$$

Acceleration gradient: $1\text{-}10\ \mathrm{TeV/m}$

Considerably **higher electron density** in a **solid state** than in a gaseous plasma

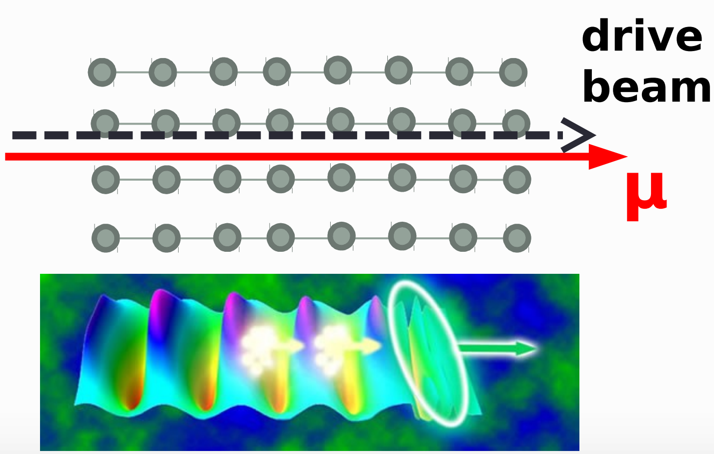
Channeling makes **crystal** almost **transparent** both to accelerated and to drive beam

Possible drive beam:

- **X-rays**
- **electrons**
- **heavy high-Z beams**

Possible accelerated beam:

- **muons**
- **e+/e-**
- **protons**



Compact muon collider?

* R. Ariniello, …, and T. Tajima, Snowmass'2021 AF6: Advanced Acceleration Concepts, arXiv: 2203.07459

T.Tajima, M.Cavenago, Crystal X-ray accelerator, Phys. Rev. Lett., 59(13), 1440 (1987).

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)

Progress of channeling physics implementation into Geant4

GEANT4

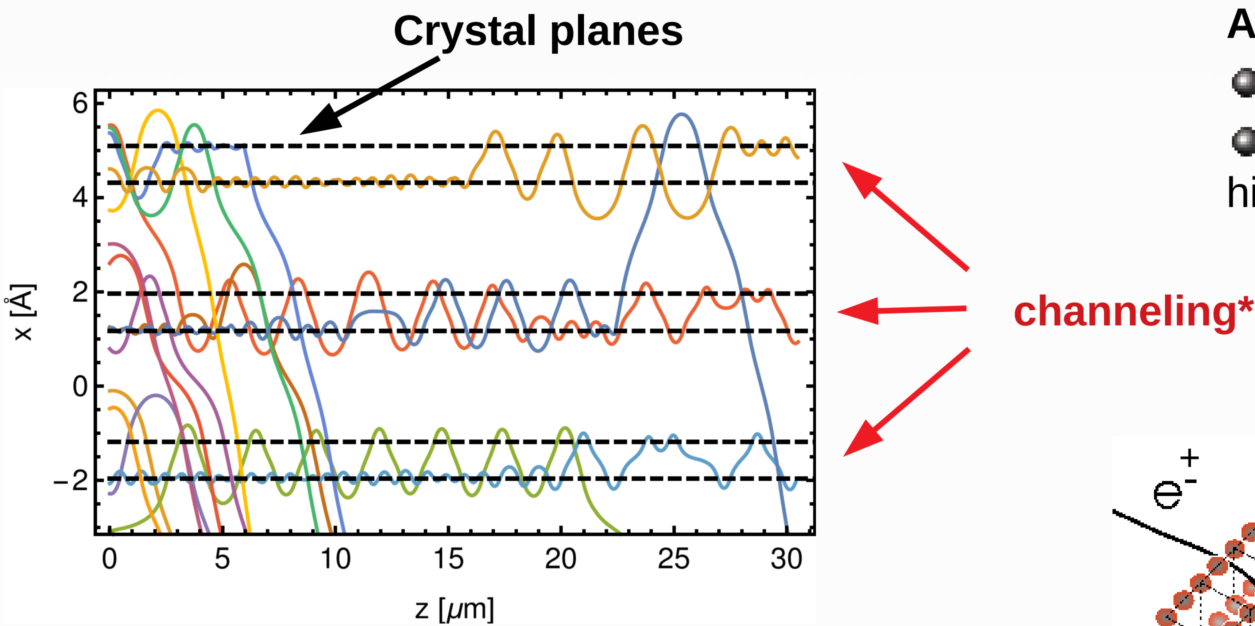
A SIMULATION TOOLKIT

Geant4 is a toolkit for the simulation of the **passage** of particles **through matter**. Its areas of application include **high energy**, **nuclear** and **accelerator physics**, as well as studies in **medical** and **space science**.

Channeling simulation technique: CRYSTALRAD Monte Carlo simulation code

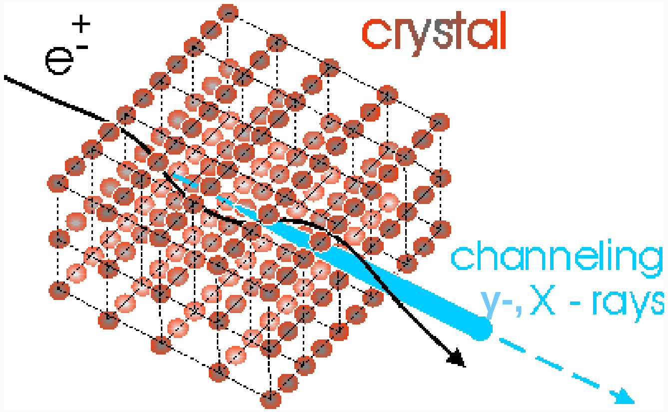
Main conception – simulation of classical trajectories of charged particles in a crystal

Multiple and single **scattering simulation** at every step



Advantages:

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

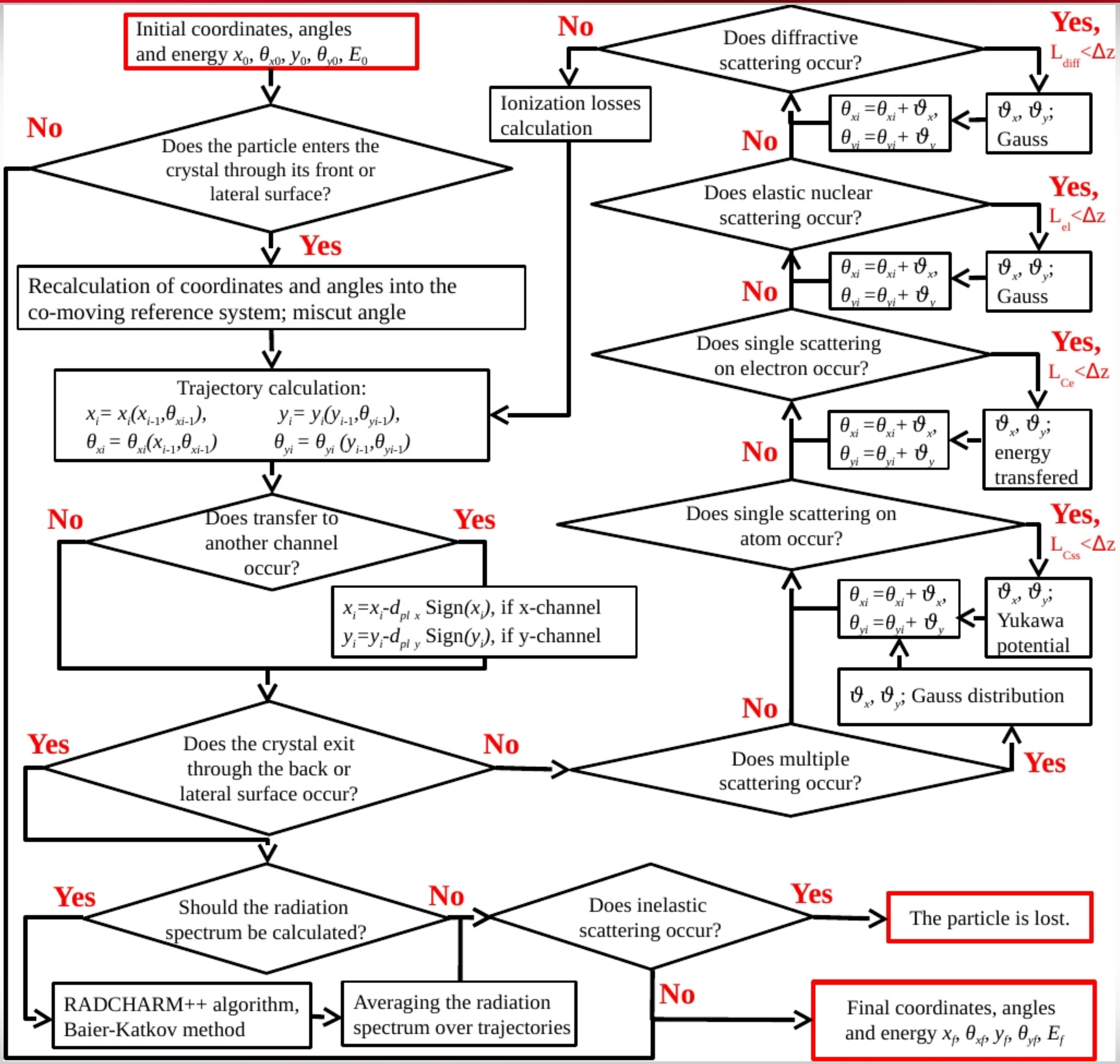


Baier-Katkov formula:
integration is made over the classical trajectory

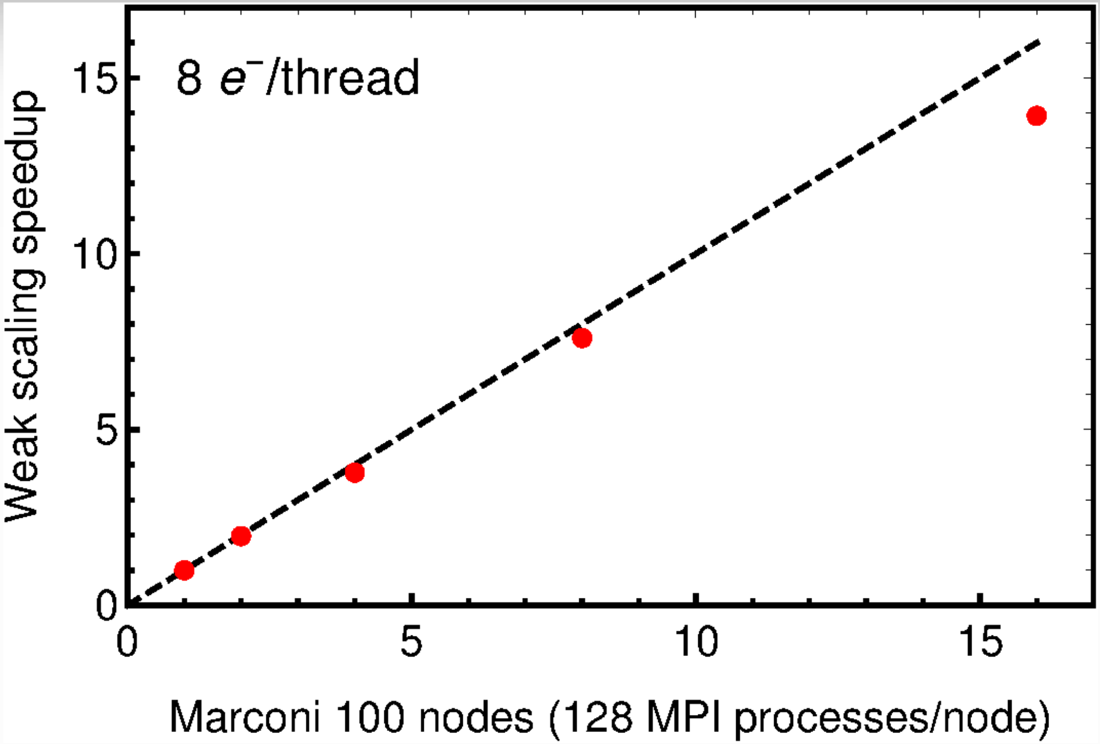
$$\frac{dE}{d^3k} = \omega \frac{dN}{d^3k} \frac{\alpha}{4\pi^2} \iint dt_1 dt_2 \frac{\left[(E^2+E'^2)(v_1 v_2 - 1) + \omega^2/\gamma^2\right]}{2E'^2} e^{-ik'(x_1 - x_2)}$$

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. arXiv: 2303.04385, Accepted for publication in JKPS**
A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

CRYSTALRAD algorithm



CRYSTALRAD weak scaling at Marconi 100@CINECA



Channeling simulations are complex and time consuming

Total nodes	Total MPI processes	electrons number	electrons/ MPI process	weak scaling speedup	execution time (s)
1	128	1024	8	1	3833
2	256	2048	8	1.97	3891
4	512	4096	8	3.77	4061
8	1024	8192	8	7.60	4033
16	2048	16384	8	13.9	4405

A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)

How to implement an external code into Geant4? Geant4 FastSim interface

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

```
G4bool TestModel::IsApplicable(const G4ParticleDefinition& particleType)
{
  return
    &particleType == G4Proton::ProtonDefinition()||
    &particleType == G4AntiProton::AntiProtonDefinition()||
    &particleType == G4Electron::ElectronDefinition() ||
    &particleType == G4Positron::PositronDefinition();// ||
    //&particleType == G4Gamma::GammaDefinition();
}

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......

G4bool TestModel::ModelTrigger(const G4FastTrack& fastTrack)
{
}

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0OOooo......

void TestModel::DoIt(const G4FastTrack& fastTrack,
                     G4FastStep& fastStep)
{
```

Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

Our project MIRACLE, no. HP10BIW7VR
Cineca Italian supercomputing center

MIRACLE, Cineca ISCRA Class B National Italian project
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 - 25/01/2023

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

Foreign organizations involved

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

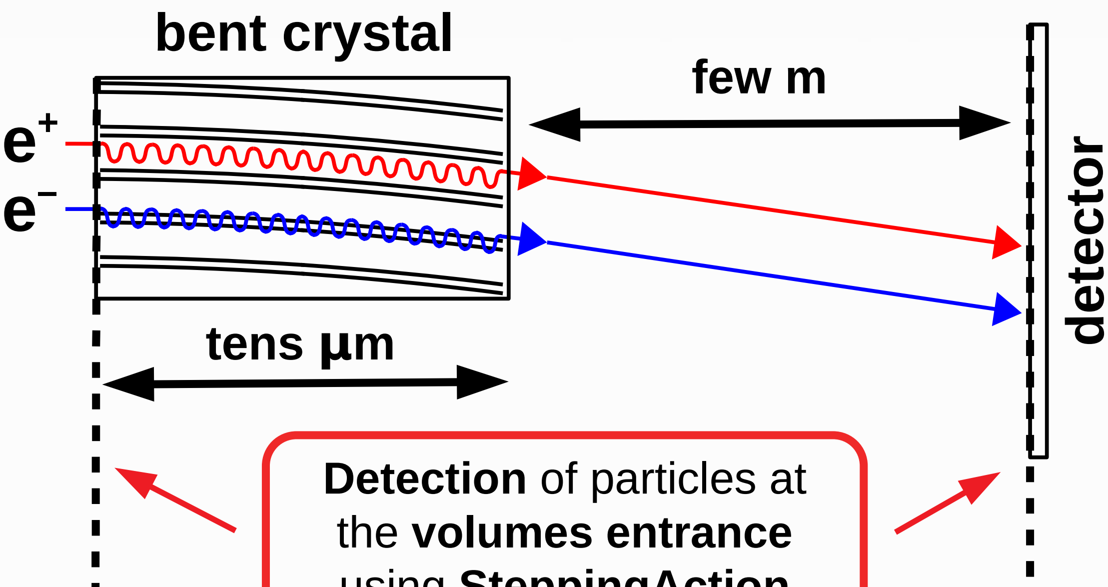
PI A. Sytov

KISTI-5 supercomputer NURION
Korea Institute of Science and Technology Information

Specification	KISTI-5 SKL
OS	CentOS 7.4
Processor	Intel Xeon Skylake (Gold 61148) 2.4GHz
Architecture	Multicore
Cores/CPU	20
CPUs/node	2
Cores/node	40
Total nodes	132
Total cores	5280

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**

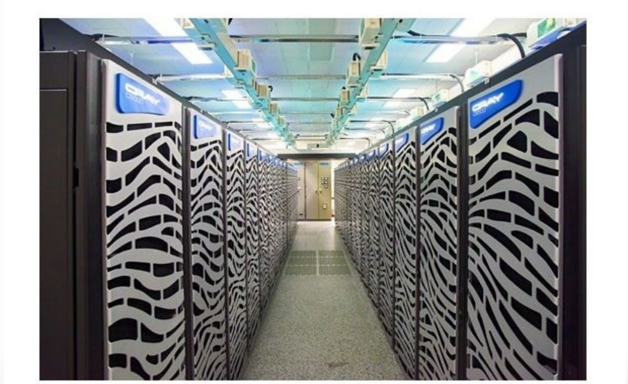


Beam setup in **run.mac** using **GPS** commands; all the **geometry** in **DetectorConstruction**

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

Detection of particles at the **volumes entrance** using **SteppingAction**

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



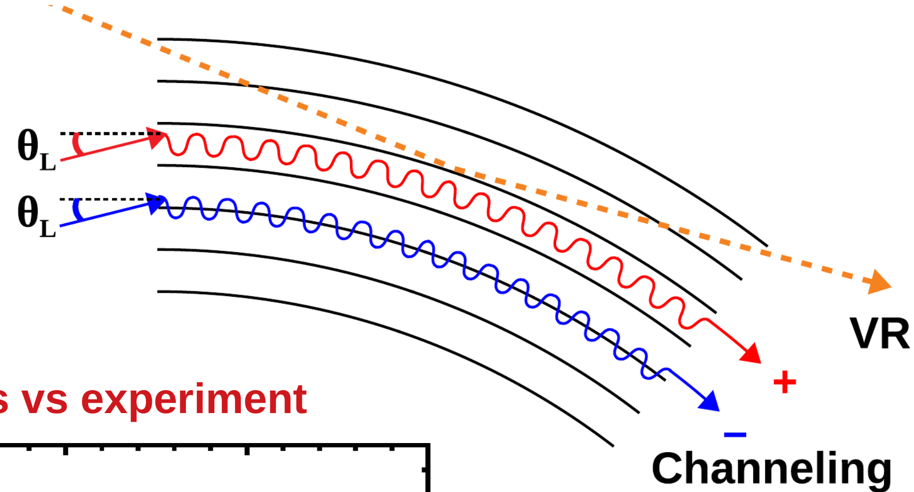
***A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)**

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

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

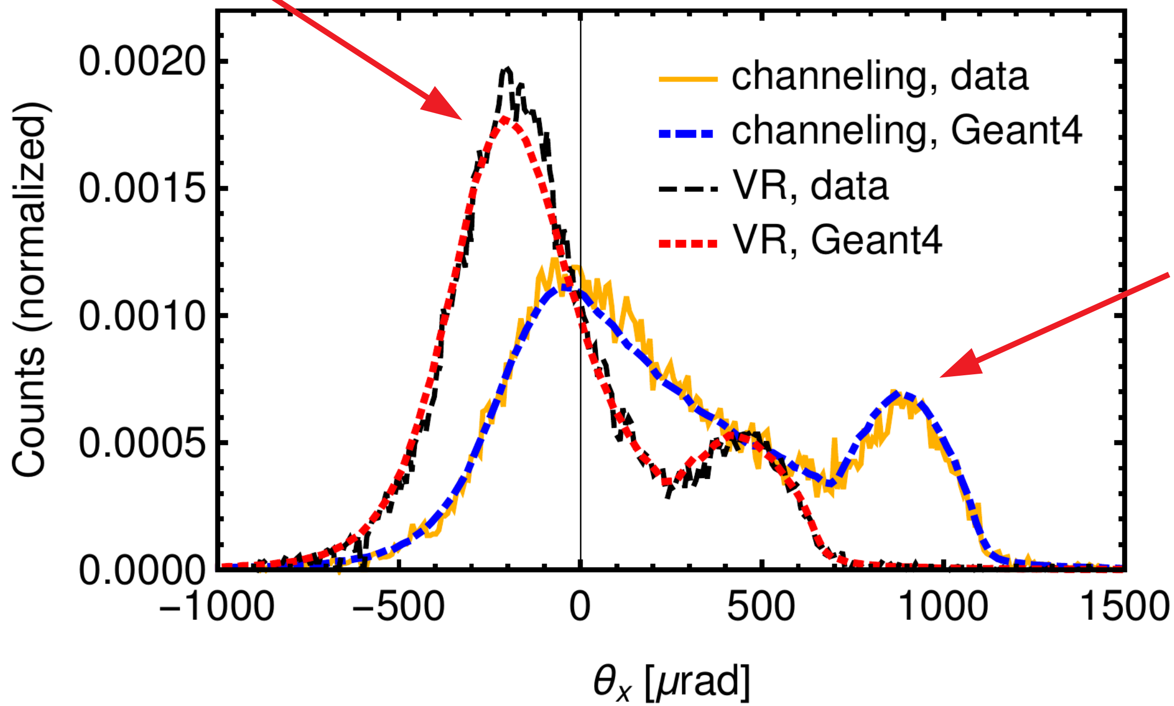
855 MeV electrons

15 µm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



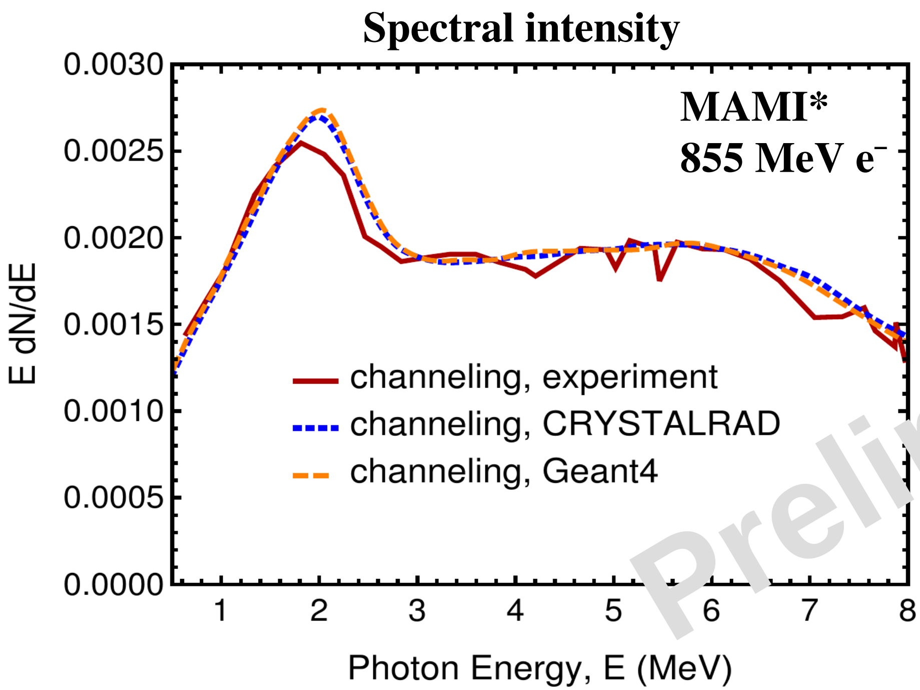
channeling

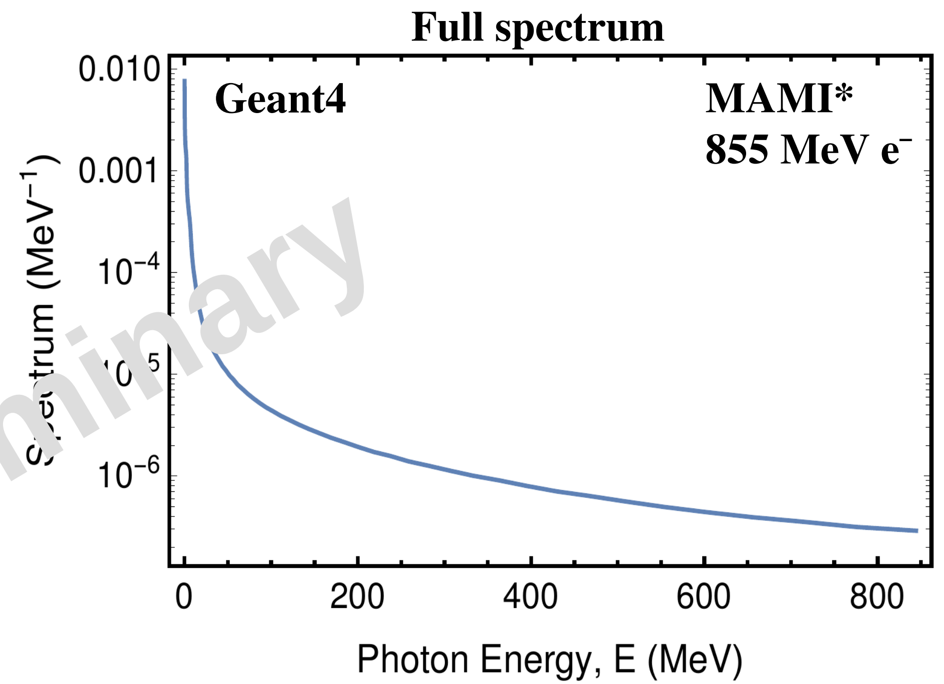
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

G4BaierKatkov:

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

Geant simulations vs experiment and CRYSTALRAD simulations





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");
            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(crystalLogic,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

Logical volume

Model activation

Additional options

Radiation model activation

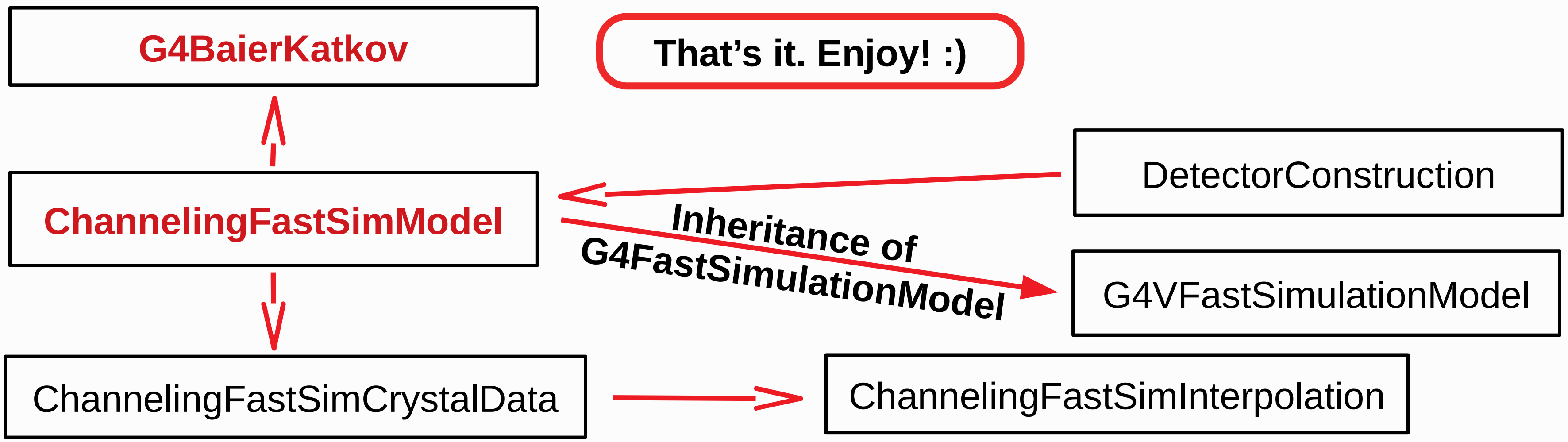
How to use the Geant4 channeling model in your example?

- **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 );
```

That's it. Enjoy! :)



Physics list independent

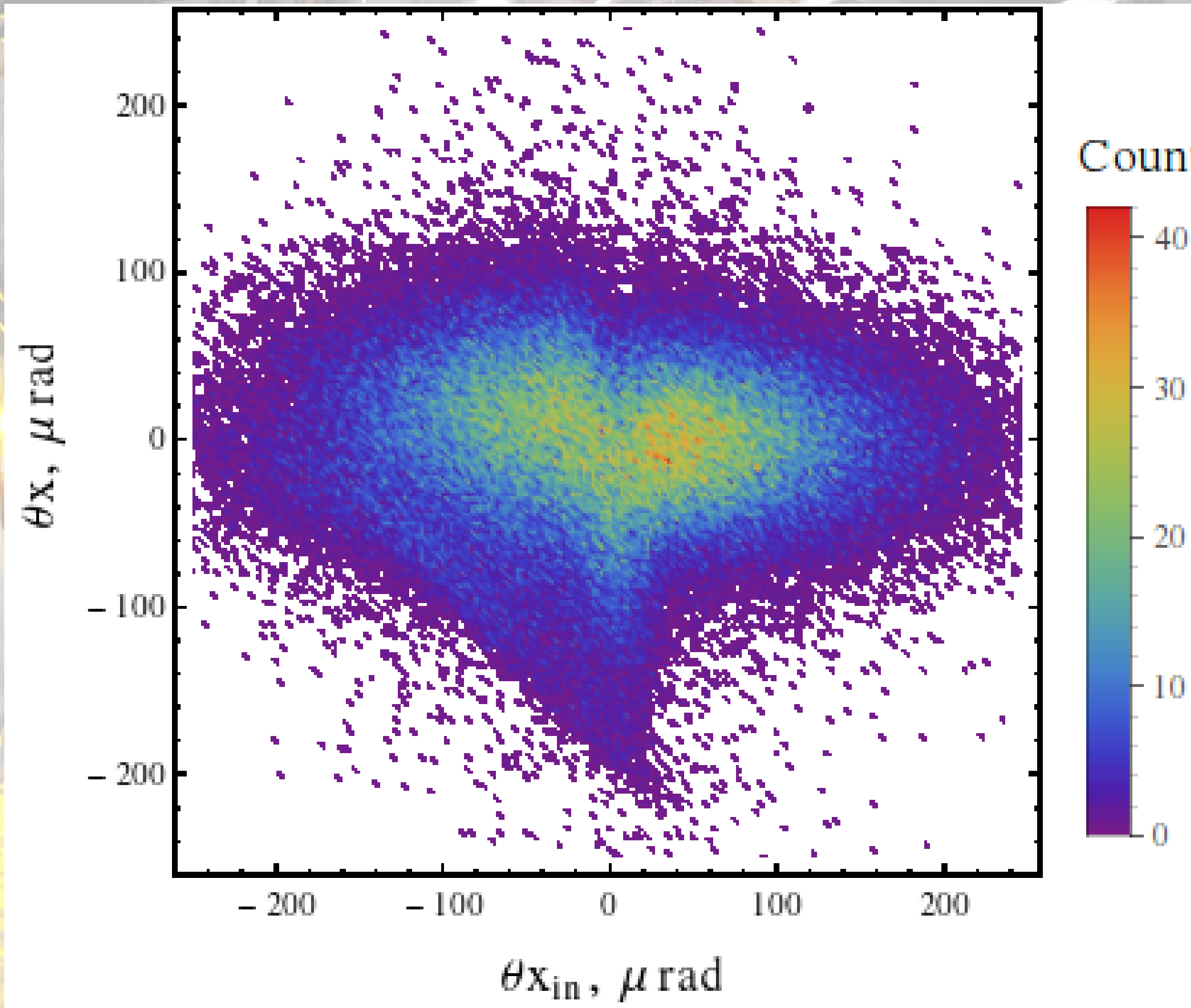
Conclusions

- 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.

- **ChannelingFastSimModel** is our implementation of channeling physics 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**.

- 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**.



Thank you for attention!