First ab-initio channeling and Baier-Katkov Geant4 FastSim model

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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:

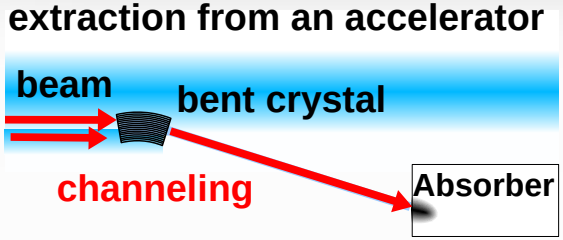
- **A. Sytov** – project coordinator
- **L. Bandiera** – INFN supervisor
- **K. Cho** – KISTI supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

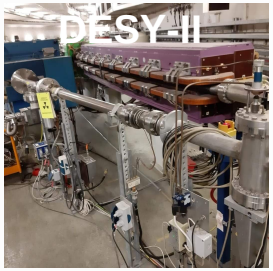
Location:

- 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)

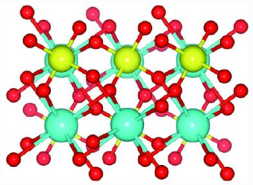
Applications*

Crystal-based collimation or beam extraction from an accelerator



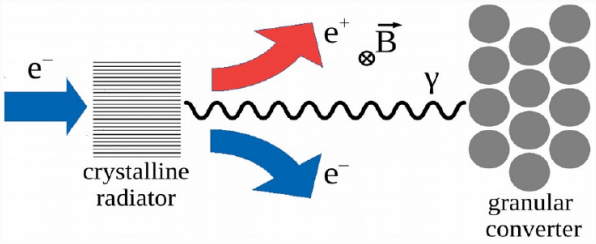


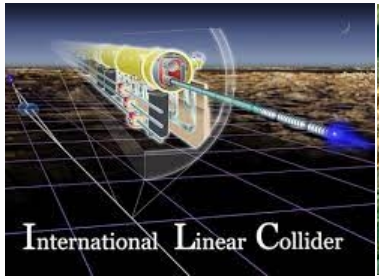
Ultrashort crystalline calorimeter



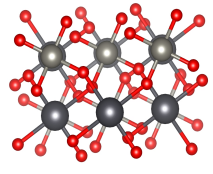
Gamma-ray Space Telescope

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

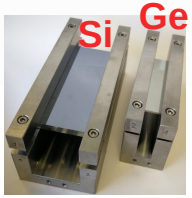




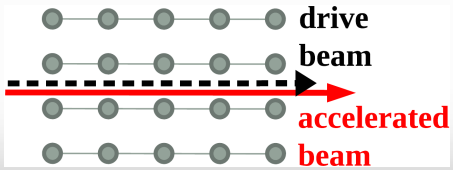
Oriented crystals



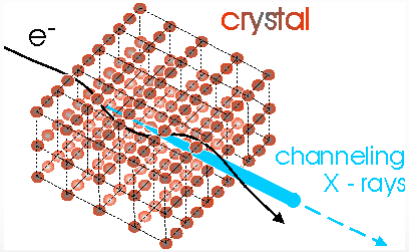
Measurement of dipole magnetic and electric moments of exotic particles

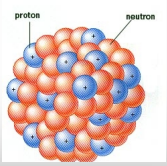


Plasma acceleration



X and y-ray source for nuclear and medical physics



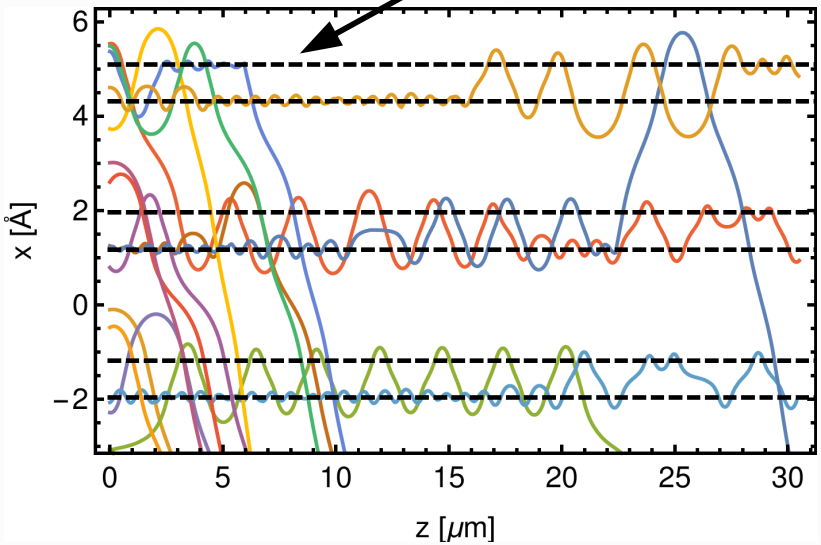


*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

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

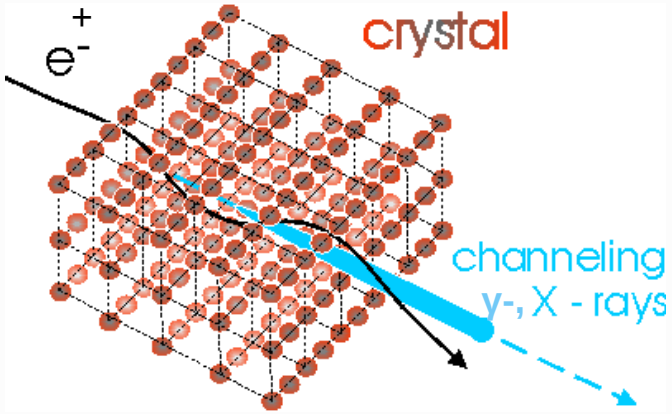
Crystal planes



channeling*

Advantages:

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



Baier-Katkov formula:

integration is made over the classical trajectory

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

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)

Why the implementation of channeling and Baier-Katkov models into Geant4 is so challenging?

Challenges of trajectory simulation

- **Complicated geometry** of crystal planes/axes especially in a bent crystal;
- **Complicated spacial structure** of cristalline **electric fields** and **atomic density** depending on the material and alignment;
- Different types of **scattering dependent** on the charge particle **positions** vs crystal planes/axes;
- **Incompatibility** of channeling with **Geant4 standard physics lists**: especially with **multiple coulomb scattering** and **bremsstrahlung** process: impossible to modify **continuous-discrete Geant4** processes during execution.

Challenges of Baier-Katkov

- Need for **recording trajectory** in order to simulate the spectrum;
- Multidimensional integral => **low simulation speed**;
- Hard gamma radiation => need to **return** the particle **back to the radiation point**, which is **not allowed in Geant4** in a simple way.

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  //....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 {
```

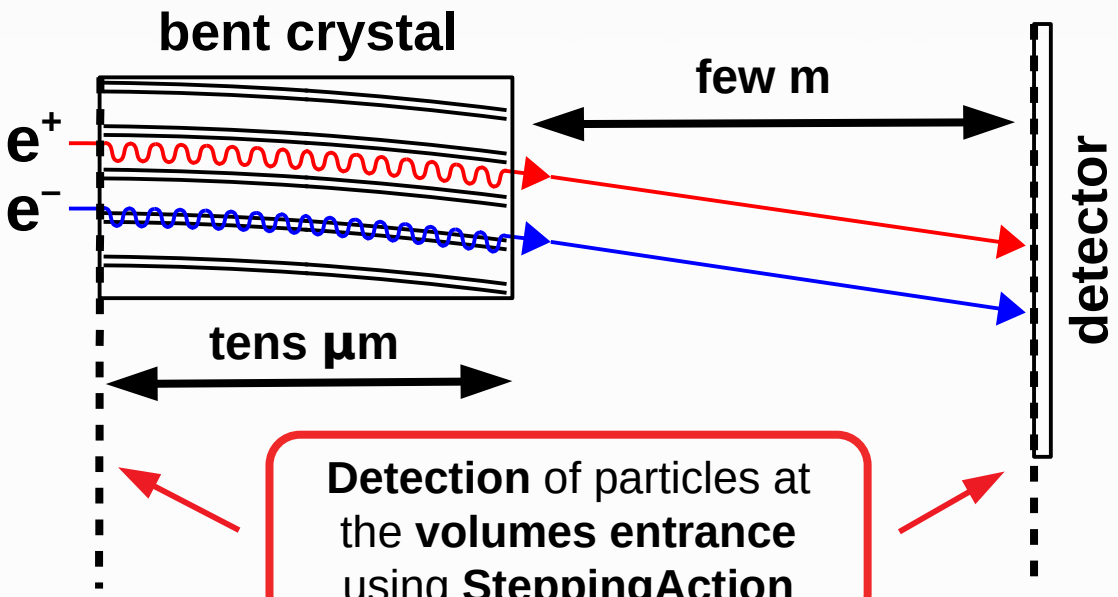
Insert particles for which the model is applicable

Insert the condition to enter the model

Insert what the model does

First Geant4 channeling example for electrons/positrons

- **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 **Galileo100@CINECA** (Italy) **NURION@KISTI** (Korea)

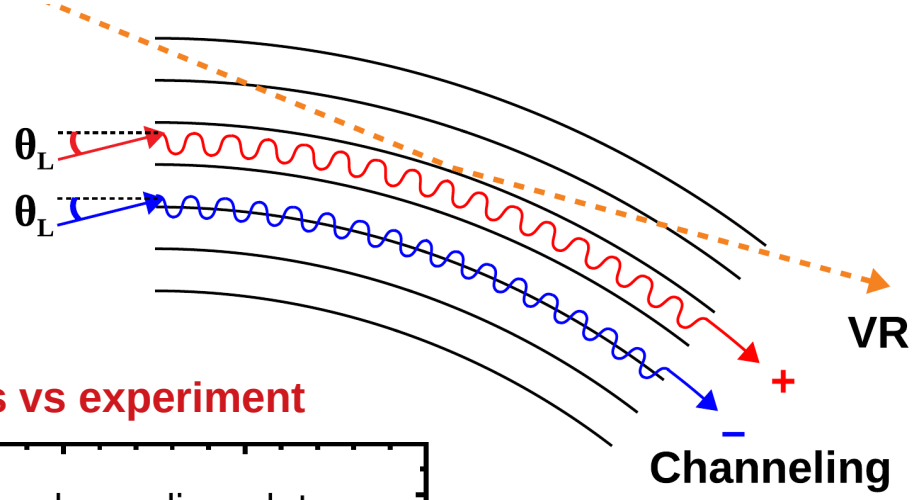
*A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

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

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

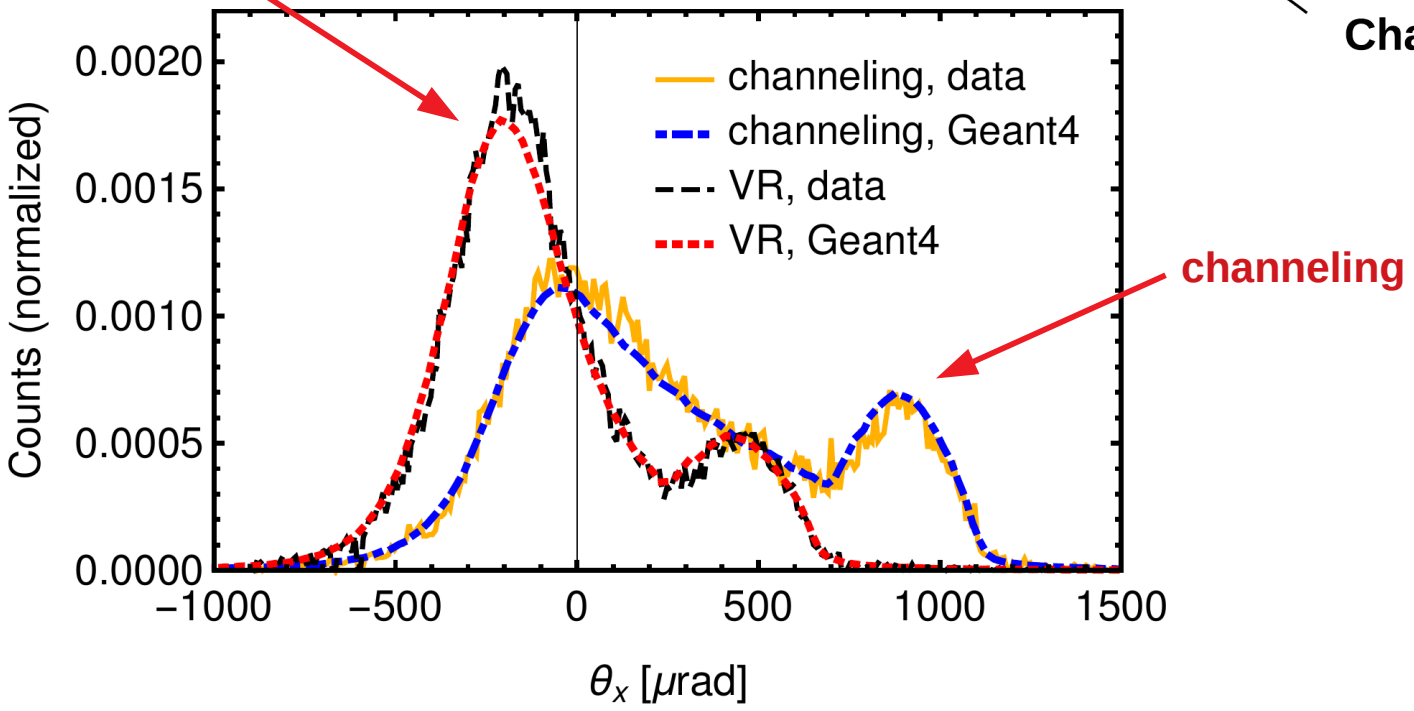
855 MeV electrons

15 μm thick bent crystal



volume reflection (VR)

Geant simulations vs experiment



channeling

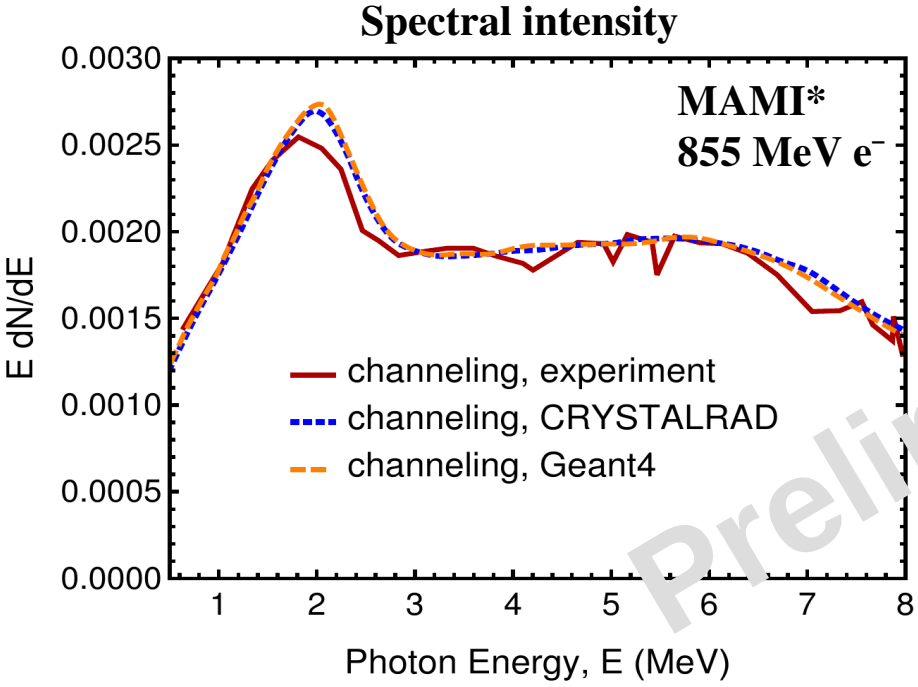
*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

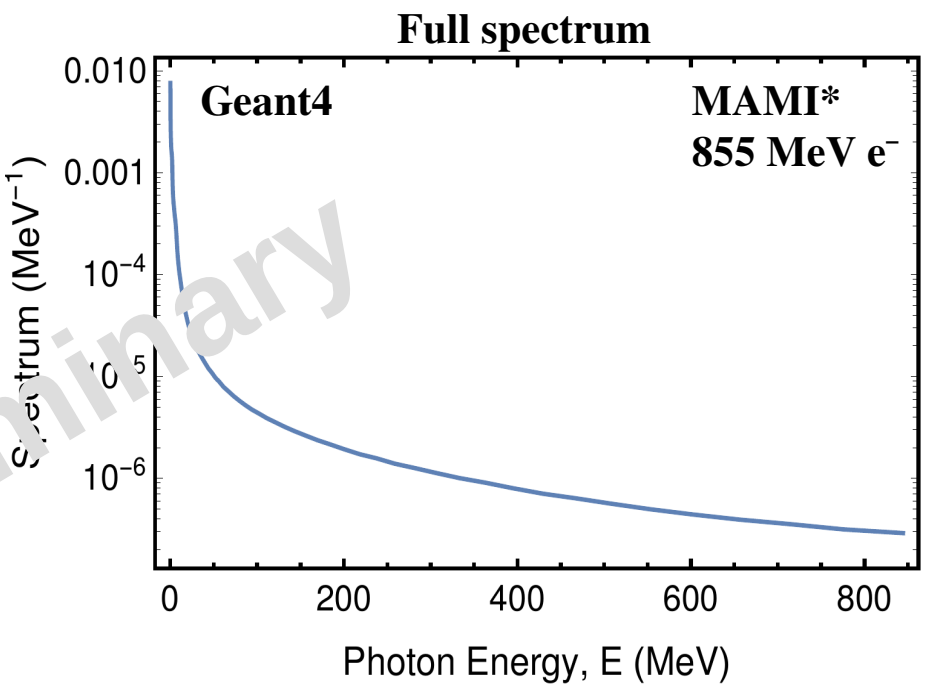
First Geant4 Baier-Katkov radiation model: radiation by 855 MeV electrons at Mainz Mikrotron MAMI*

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**

Geant simulations vs experiment and CRYSTALRAD simulations





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

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.);
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

- **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
    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

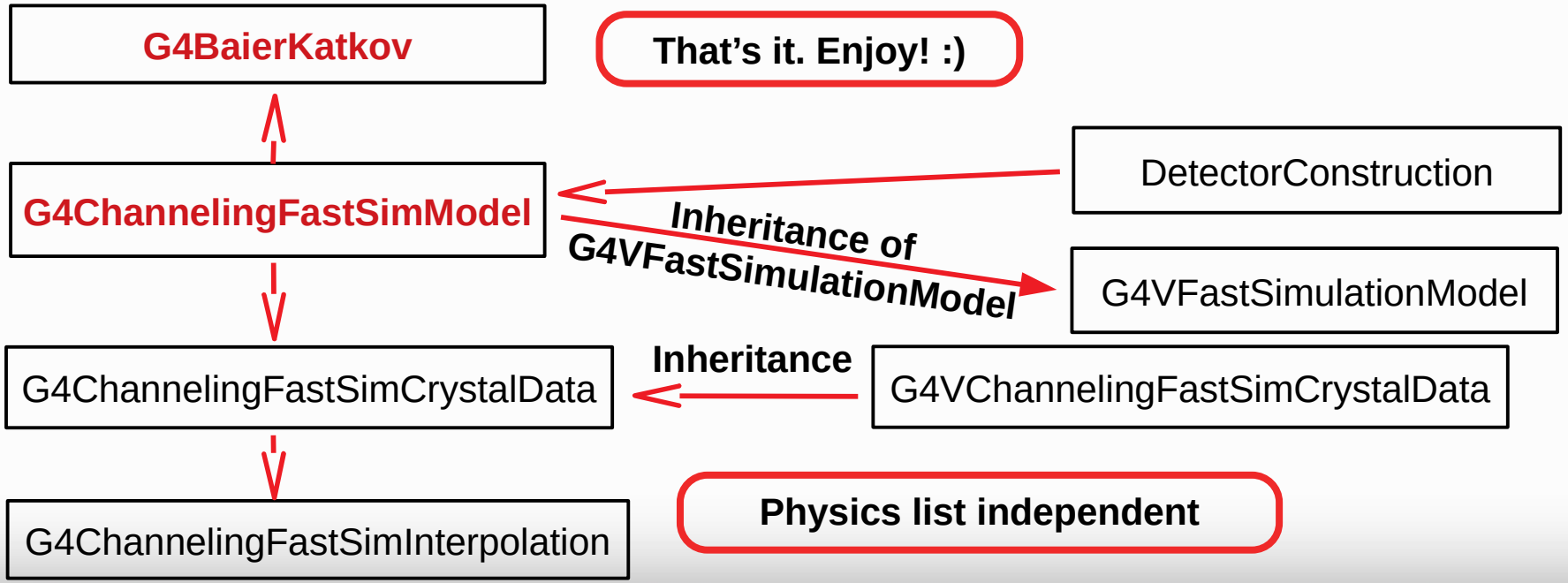
Radiation model activation

How to use the Geant4 channeling model in your example?

- **Add to main:**

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 );
```



Current status

Submitted into Geant4 kernel!

Please use it!

Don't hesitate to contact me in the case of any problems/issues/suggestions
sytov@fe.infn.it

Please cite our papers if you use our model:

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

Future plans

- **Extensive validation of channeling** model and **Baier-Katkov** model: **2023**

You can help us with that!

- To **submit** an updated version into **Geant4 annual release** **END OF 2023**
- **Coherent pair production** model (**V. Haurylavets** talk) **IN PROGRESS**
- **Radiation** and **positron source examples** **2023-2024**
- **Beam extraction example** **2024**

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.

- **G4ChannelingFastSimModel** is our implementation of channeling physics and Baier-Katkov method 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**.

- **G4ChannelingFastSimModel and G4BaierKatkov** models were submitted into the **Geant4 kernel** in the next beta-release.

- 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**.

Acknowledgments

Marie Sklodowska-Curie Action Global Individual Fellowships TRILLION (G.A. 101032975) is in synergy with the following projects I would like to acknowledge:

- **MC-INFN** project (INFN Geant4 group);
- **INFN OREO** project;
- **INFN GALORE** project;
- **H2020-MSCA-RISE N-LIGHT** (G.A. 872196) and **EIC-PATHFINDER-OPEN TECHNO-CLS** (G.A. 101046458) projects.
- We acknowledge the **CINECA** award under the **ISCRA** initiative, for the availability of high-performance computing resources and support.
- This work is also supported by the Korean National Supercomputing Center with supercomputing resources including technical support (**KSC-2022-CHA-0003**).

I also thank the **Geant4 collaboration** members, in particular:

Prof. Vladimir Ivanchenko (**CERN**), **Prof. Pablo Cirrone and Dr. Luciano Pandola** (**INFN LNS**), **Prof. Kihyeon Cho, Prof. Soonwook Hwang** and **Dr. Kyungho Kim** (**KISTI**), **Prof. Susanna Guatelli** and **Prof. Anatoly Rosenfeld** (**University of Wollongong**), **Dr. Gianfranco Paternò (INFN Ferrara) as well as Prof. Makoto Asai (Jlab) and Prof. Marc Verderi (IN2P3/LLR)** for fruitful collaboration and discussions!

감사합니다 !