A. Sytov
On behalf of INFN Ferrara team

CHANNELING MODEL IN GEANT4

MC-INFN/GEANT4 meeting, April 21, 2021

Outline: past, present and future

Milestones 2020:

- **Comparison** between **Geant4** simulations and **experimental** data as well as simulations by the **CRYSTALRAD** simulation code.
- Proposal of **Geant4 channeling model improvements**.

Milestones 2021:

- Inclusion of the **Baier-Katkov method** for computation of radiation in oriented crystals into Geant4 and comparison with **experimental data**.
- Geant4 **channeling** and **channeling radiation model improvements**.

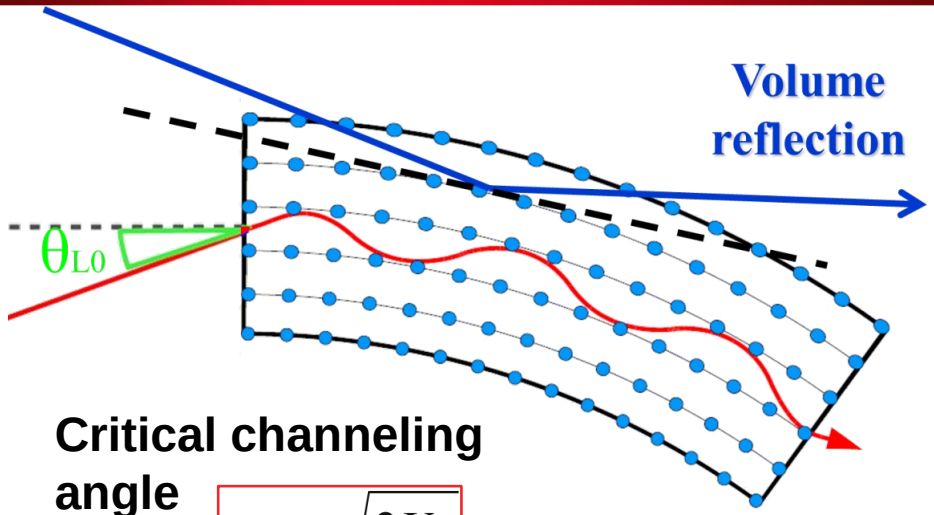
CINECA ISCRA Class B Project for CPU time 2020-2021:

- Project **LEADER** “Electron crystal-based extraction”

Marie Sklodowska-Curie Action Global Fellowships 2021-2024:

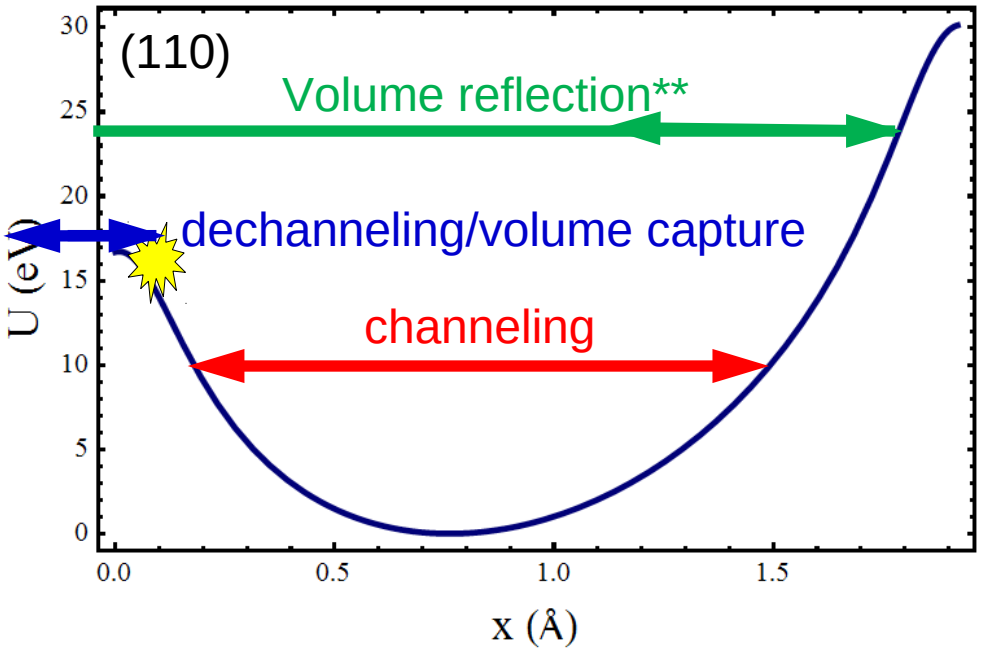
- Project **TRILLION** “Steering and radiation effects in oriented crystals and their applications implementation into Geant4”

Channeling and volume reflection in a bent crystal*



Critical channeling angle

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



Pecularities of channeling simulations:

- Very **small steps ~ nm-μm**
- The next step depends on the previous one
- **Multiple scattering** makes the trajectory stochastic
- **Strong single scattering** may be crucial

No channeling cross-section,
Channeling effect is complicated

Standard **Coulomb scattering** models **may be invalid** at small steps

***E.N. Tsyganov, Fermilab TM-682 (1976)**

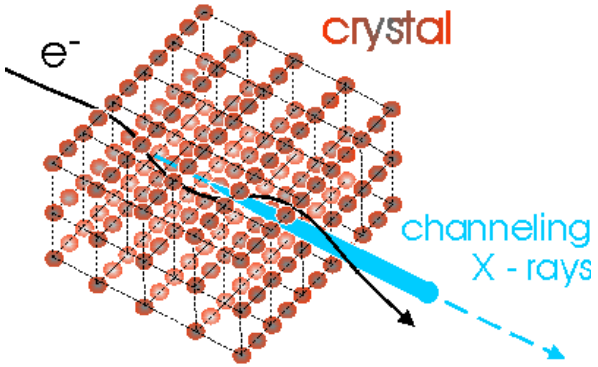
****A.M. Taratin, S.A. Vorobiev, NIM B 26, 512 (1987)**

Introduction Baier-Katkov algorithm from CRYSTALRAD into Geant4 to simulate channeling radiation

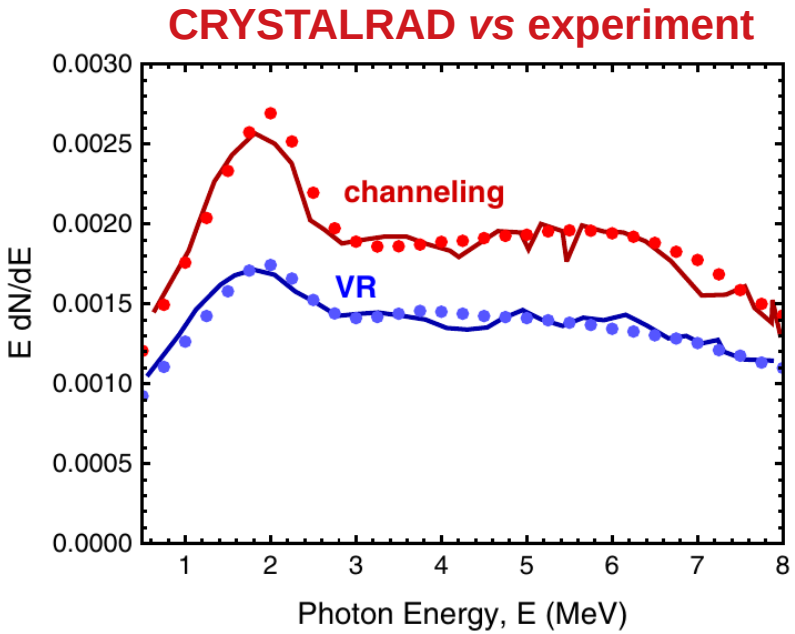
The electromagnetic radiated energy is evaluated with **the Baier-Katkov formula** **

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

where the integration is made over the classical trajectory.



The **Baier-Katkov** method permits to simulate the emitted radiation in crystals in a wide energy range, from **sub-GeV** to **hundreds** of **GeV**.



***L. Bandiera, et al., Nucl. Instrum. Methods Phys. Res., Sect. B 355, 44 (2015)**
****V.N. Baier, V.M. Katkov, V.M. Strakhovenko World Scientific, Singapore (1998)**
*****V. Guidi, L. Bandiera, V. Tikhomirov, Phys. Rev. A 86 (2012) 042903**
******A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. PRAB 22, 064601 (2019)**

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**

New: unification of the **CRYSTAL*** code developed by **A. Sytov** and the **RADCHARM++**** code developed by **L. Bandiera** into the **CRYSTALRAD***** code to simulate the radiation spectra by **Baier-Katkov** formula

Advantages:

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

What have we been granted by (2016-2020)?

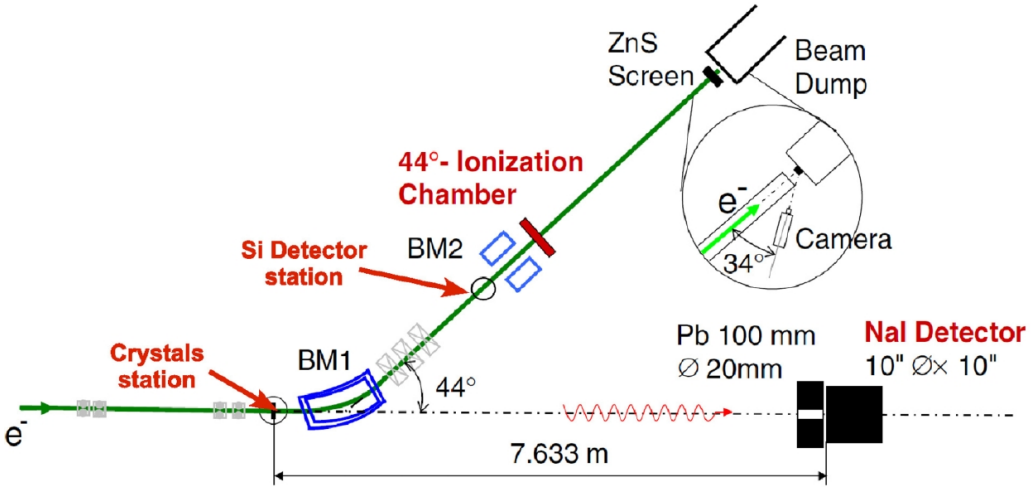
- **FERMI: 200 kh**
- **GALILEO: 500 kh**
- **MARCONI: 2.4 Mh**

***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)**

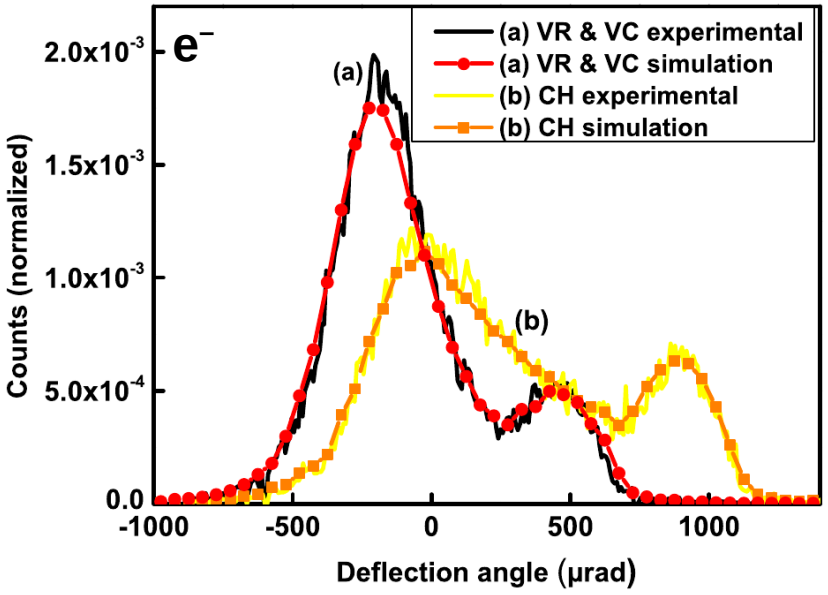
Preliminary results: Geant4 simulation of channeling of 855 MeV electrons at Mainzer Mikrotron MAMI



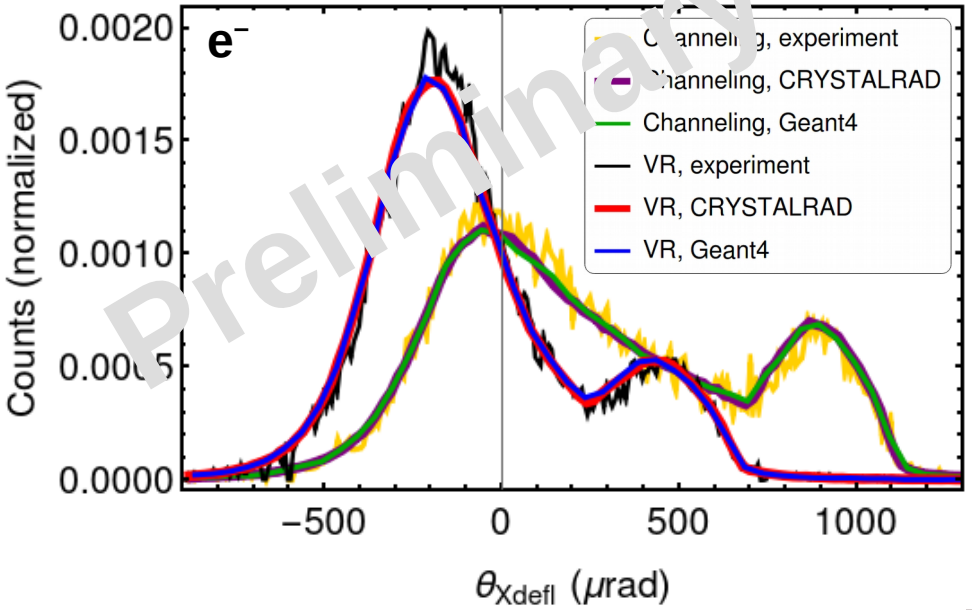
Simulation parameters

- Silicon crystal **30.5 µm** thick
- Planes: **(111)**
- Electron beam **855 MeV**
- Beam divergence **30 µrad**

Results published in 2014*



Geant simulations vs experiment and CRYSTALRAD simulations



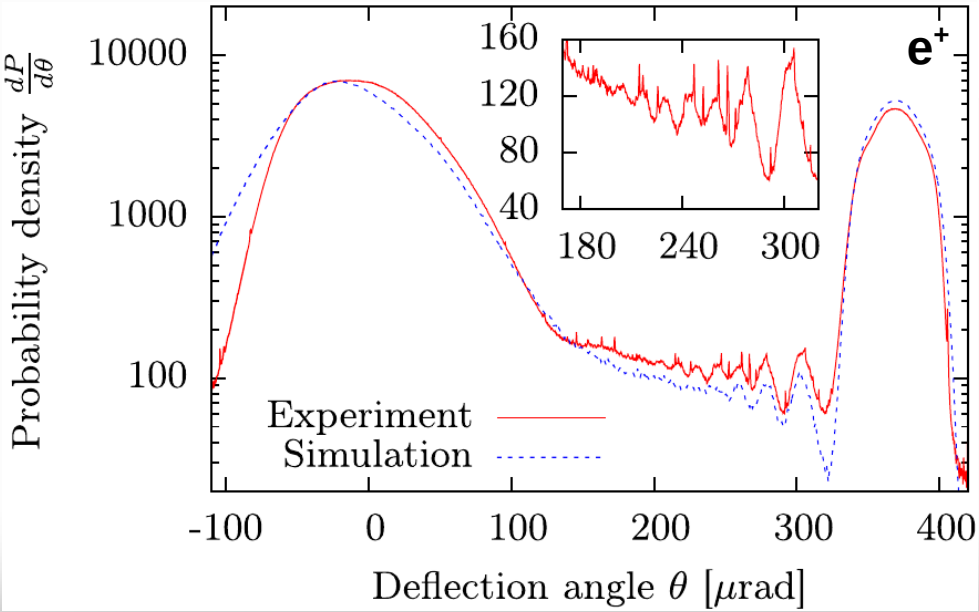
A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

Preliminary results: Geant4 simulation of the effect of quasichanneling oscillations observed at SLAC FACET for 20.35 GeV e^+/e^-

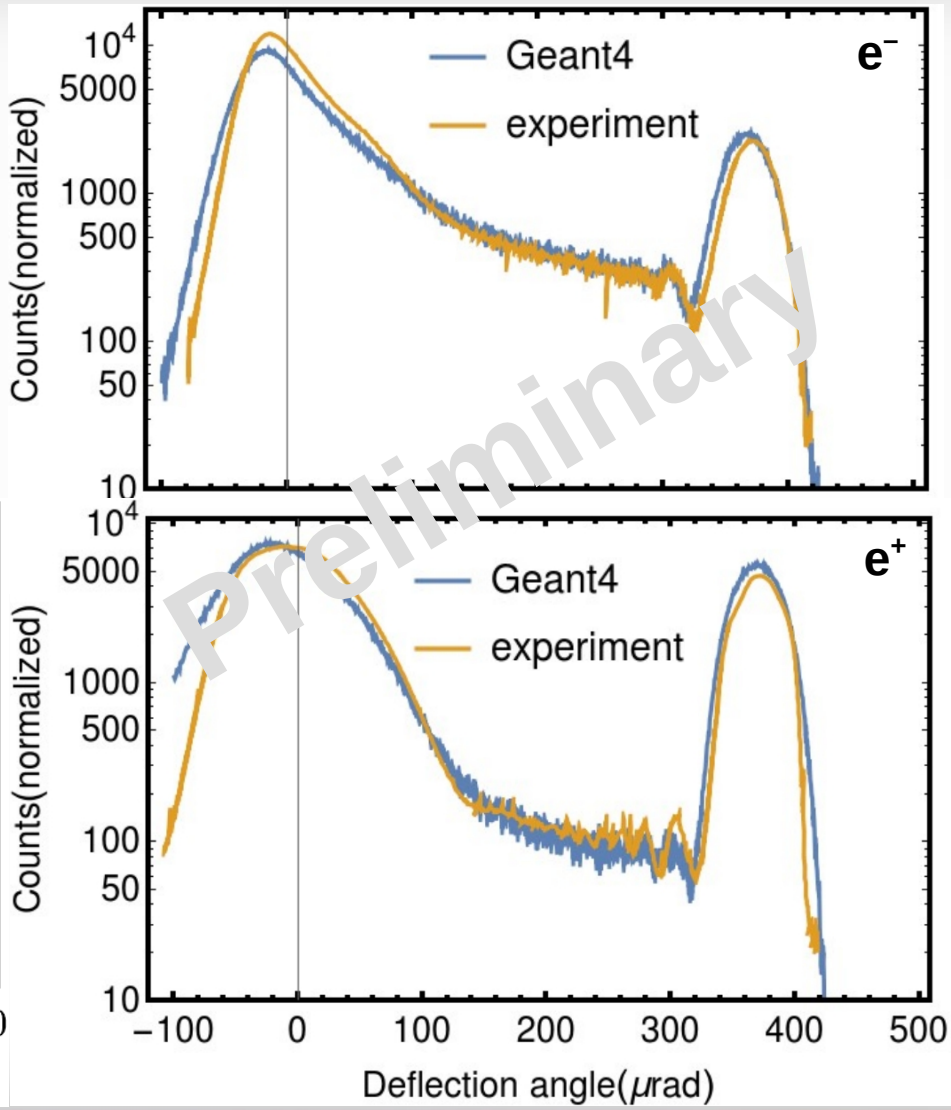
Quasichanneling oscillations in the deflection angle distributions, the effect **predicted by A. Sytov***

***A.I. Sytov et al. Eur. Phys. J. C 76, 77 (2016)**

CRYSTAL simulations *vs* experiment published in 2017*



Geant simulations *vs* experiment



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

Validation of simulations and articles published

Experimental validation of our simulation model for protons, electrons and positrons

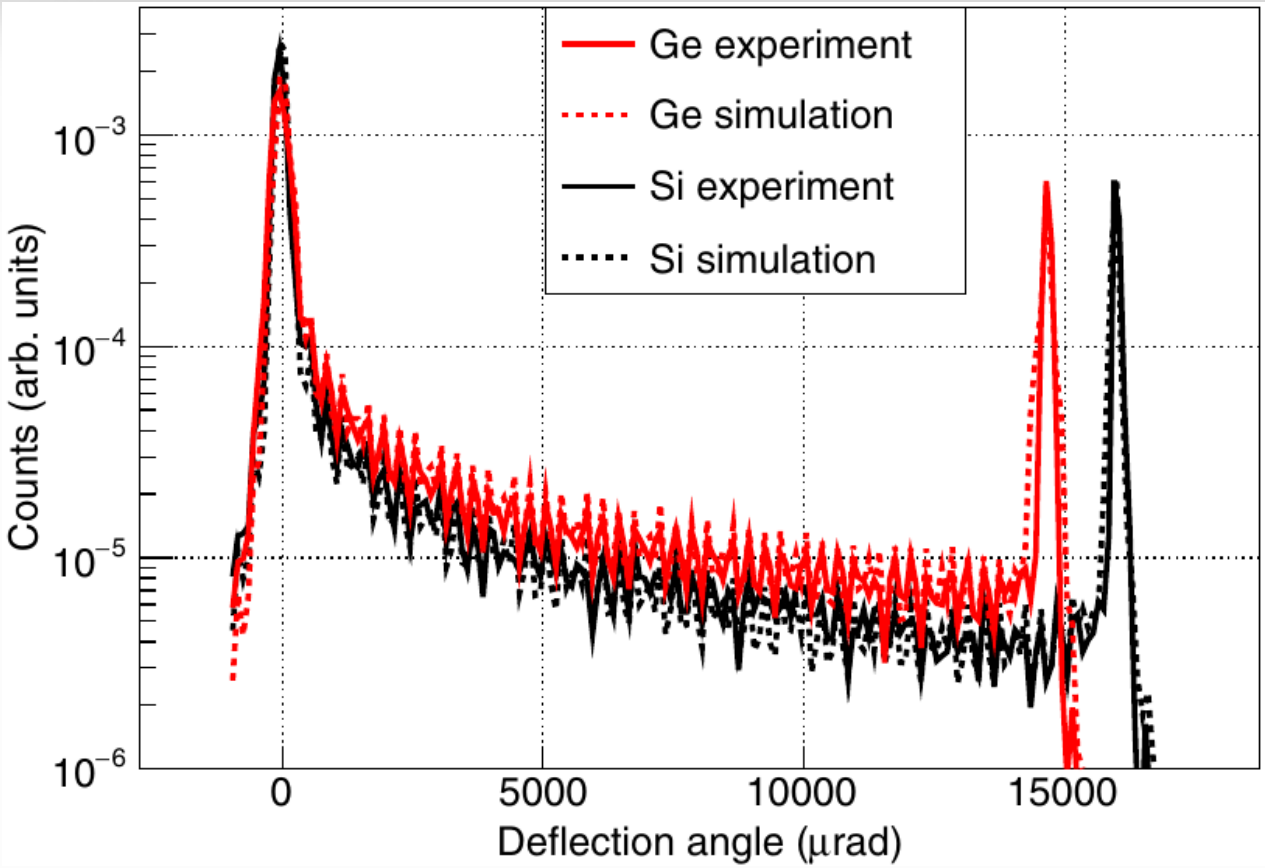
A. Mazzolari, A. Sytov et al. **Eur. Phys. J. C** 80, 63 (2020)
A. I. Sytov, V. V. Tikhomirov, and L. Bandiera. **Phys. Rev. Acc. and Beams** 22, 064601 (2019)
T. N. Wistisen, …, and A. Sytov. **Phys. Rev. Lett.** 119, 024801 (2017)
A. I. Sytov et al. **Eur. Phys. J. C** 77, 901 (2017)
A.I. Sytov, V.V. Tikhomirov. **NIM B** 355 (2015) 383–386.
L. Bandiera et al. **Phys. Rev. Lett.** 115, 025504 (2015)
A. Mazzolari et al. **Phys. Rev. Lett.** 112, 135503 (2014)
V. Guidi, L. Bandiera and V. Tikhomirov, **Phys. Rev. A** 86, 042903 (2012)
L. Bandiera et al. **Phys. Rev. Lett.** 111, 255502 (2013)
V. Guidi, A. Mazzolari and V. Tikhomirov, **J. of Appl. Phys.** 107, 114908 (2010)

NEW in the frame of MC-INFN:
S. Aiola et al. Phys. Rev. D 103, 072003 (2021)
L. Bandiera, A. Sytov et al. Eur. Phys. J. C 81, 284 (2021)

Experiments for which we do simulations

- INFN ELIOT, INFN STORM
- SELDOM, Horizon 2020 n. 771642
- PEARL Project, H2020-MSCA-RISE-2015 call, n. 690991

Geant4 simulation of SELDOM experiment at CERN SPS H8 on 180 GeV protons and pions channeling in long Si and Ge bent crystals

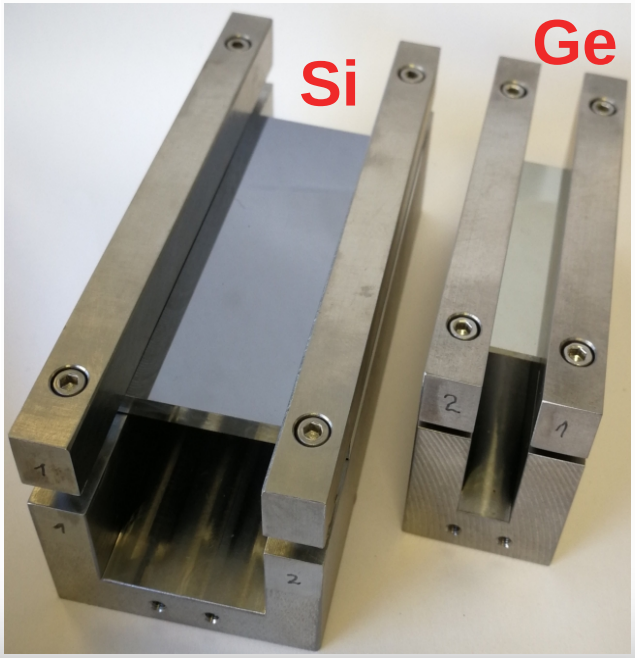


Si

- length: **8 cm**
- bending angle: **16 mrad**
- planes: **(111)**

Ge

- length: **5.5 cm**
- bending angle: **14.7 mrad**
- planes: **(110)**



Simulation of complete setup
Not only the crystal

Problem with the class **G4ChannelingOptrChangeCrossSection**

```
77  void G4ChannelingSOptrChangeCrossSection::StartRun(){
78      if ( fSetup ){
79          const G4ProcessManager* processManager = fParticleToBias->GetProcessManager();
80          const G4BiasingProcessSharedData* sharedData =
81          G4BiasingProcessInterface::GetSharedData( processManager );
82          if ( sharedData ){
83              for ( size_t i = 0 ; i < (sharedData->GetPhysicsBiasingProcessInterfaces()).size(); i++ ){
84                  const G4BiasingProcessInterface* wrapperProcess =
85                  (sharedData->GetPhysicsBiasingProcessInterfaces())[i];
86                  G4String processName = wrapperProcess->GetWrappedProcess()->GetProcessName();
87                  G4String operationName = "channelingChangeXS-" + processName;
88                  fChangeCrossSectionOperations[wrapperProcess] =
89                  new G4BOptnChangeCrossSection(operationName);
90
91                  G4ProcessType type = wrapperProcess->GetWrappedProcess()->GetProcessType();
92                  G4int subType = wrapperProcess->GetWrappedProcess()->GetProcessSubType();
93
94                  switch (type) {
95                      case fNotDefined:
96                          fProcessToDensity[processName] = fDensityRatioNone;
97                          break;
98                      case fTransportation:
99                          fProcessToDensity[processName] = fDensityRatioNone;
100                         break;
101                     case fElectromagnetic:
102                         if(subType == fCoulombScattering ||
103                            subType == fMultipleScattering){
104                             fProcessToDensity[processName] = fCancelProcess;
105                         }
106                         if(subType == fIonisation ||
107                            subType == fBremsstrahlung){
108                             fProcessToDensity[processName] = fCancelProcess;
109                         }
110                         if(subType == fPairProdByCharged ||
111                            subType == fAnnihilation ||
112                            subType == fAnnihilationToMuMu ||
113                            subType == fAnnihilationToHadrons){
```

It is not possible to turn off/to modify **continuous discrete processes** (multiple scattering, ionization losses) in this way but **discrete processes**

First solution: G4Region

- Modification of the energy range of the process inside the volume in the physics list.
- By now done only for **G4hMultipleScattering**, to do for **G4hIonisation**; **G4eBremsstrahlung** etc.
- **Is it possible to turn off/turn on continuous discrete processes on every Geant4 step inside a volume? This is the main difficulty of the project**

```
} else if (particleName == "proton" ||
           particleName == "anti_proton") {

  G4hMultipleScattering* pmsc = new G4hMultipleScattering();
  pmsc->AddEmModel(1,new G4WentzelVIModel());
  G4hIonisation* hIoni = new G4hIonisation();

  ph->RegisterProcess(pmsc, particle);
  //ph->RegisterProcess(hIoni, particle);
  //ph->RegisterProcess(pb, particle);
  //ph->RegisterProcess(pp, particle);
  ph->RegisterProcess(new G4CoulombScattering(), particle);

  G4WentzelVIModel* msk2 = new G4WentzelVIModel();
  msk2->SetActivationHighEnergyLimit(100*MeV);
  em_config->SetExtraEmModel(particleName,"msc",msk2,"Target",0.0,100*MeV);
```

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Dedicated supercomputer time on Marconi-100: project LEADER, Cineca ISCRA Class B National Italian project, no. HP10BHSQLS

```
**********************************************************************************
* Welcome to MARCONI100 Cluster /                                                *
*            IBM Power AC922 (Whiterspoon) -                                     *
*            Red Hat Enterprise Linux Server release 8.1 (Ootpa)                 *
*                                                                                *
* 980 compute nodes with:                                                        *
*       - 2x16 cores IBM POWER9 AC922 at 3.1 GHz                                 *
*       - 4 x NVIDIA Volta V100 GPUs, Nvlink 2.0, 16GB                           *
*       - 256 GB RAM                                                             *
```

1.5 Mh for 1 year

Main goal: simulation of electron beam crystal-based extraction from the DESY-II synchrotron

PI A. Sytov

One scope of the project is simulations the development of radiation loss model: **synergy with MC-INFN**

Project collaborators

INFN Section of Ferrara
- Dr. Laura Bandiera
- Prof. Vincenzo Guidi
- Dr. Andrea Mazzolari
- Mattia Soldani

DESY
- Dr. Gero Kube

INFN, Laboratori Nazionali del Sud
- Prof. Pablo Cirrone

Institute for Nuclear Problems, Minsk, Belarus
- Viktar Haurylavets
- Prof. Victor Tikhomirov

Ask me if you need CPU time!

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

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
- **M. Asai** – SLAC supervisor
- **G. Kube** – DESY supervisor
- **I. Chaikovska** – IJCLab Orsay supervisor

Location:

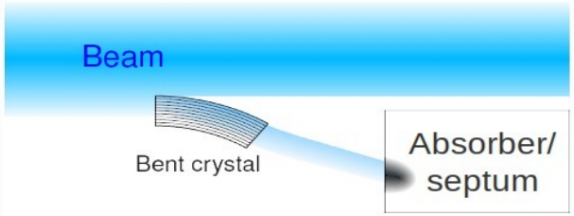
- 2 years at **SLAC** (partner organization).
- 1 year at **INFN Section of Ferrara** (host organization).
- 1 month of secondment at **DESY** (partner organization).
- 1 month of secondment at **IJCLab Orsay** (partner organization).

We thank the **MC-INFN** project for the support!

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

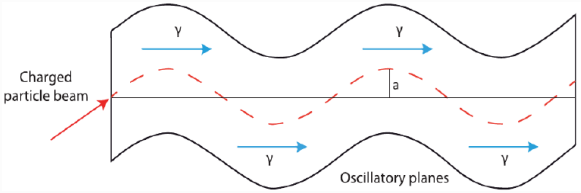
Specific applications to implement into Geant4:

- **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.



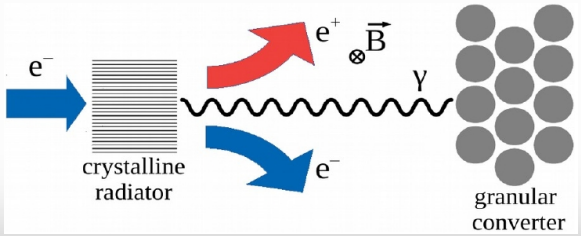
Directly connected with CINECA Project **LEADER**

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



Directly connected with milestones 2021 of **MC-INFN** as well as INFN **ELIOT** and **STORM**; European Commission **N-LIGHT** and **PEARL** projects

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



MC-INFN and **LEADER** goals are necessary preparisons for **TRILLION** which will help to accomplish INFN **ELIOT** and **STORM** as well as **N-LIGHT** **=> synergy of projects**

Conclusions: past, present and future

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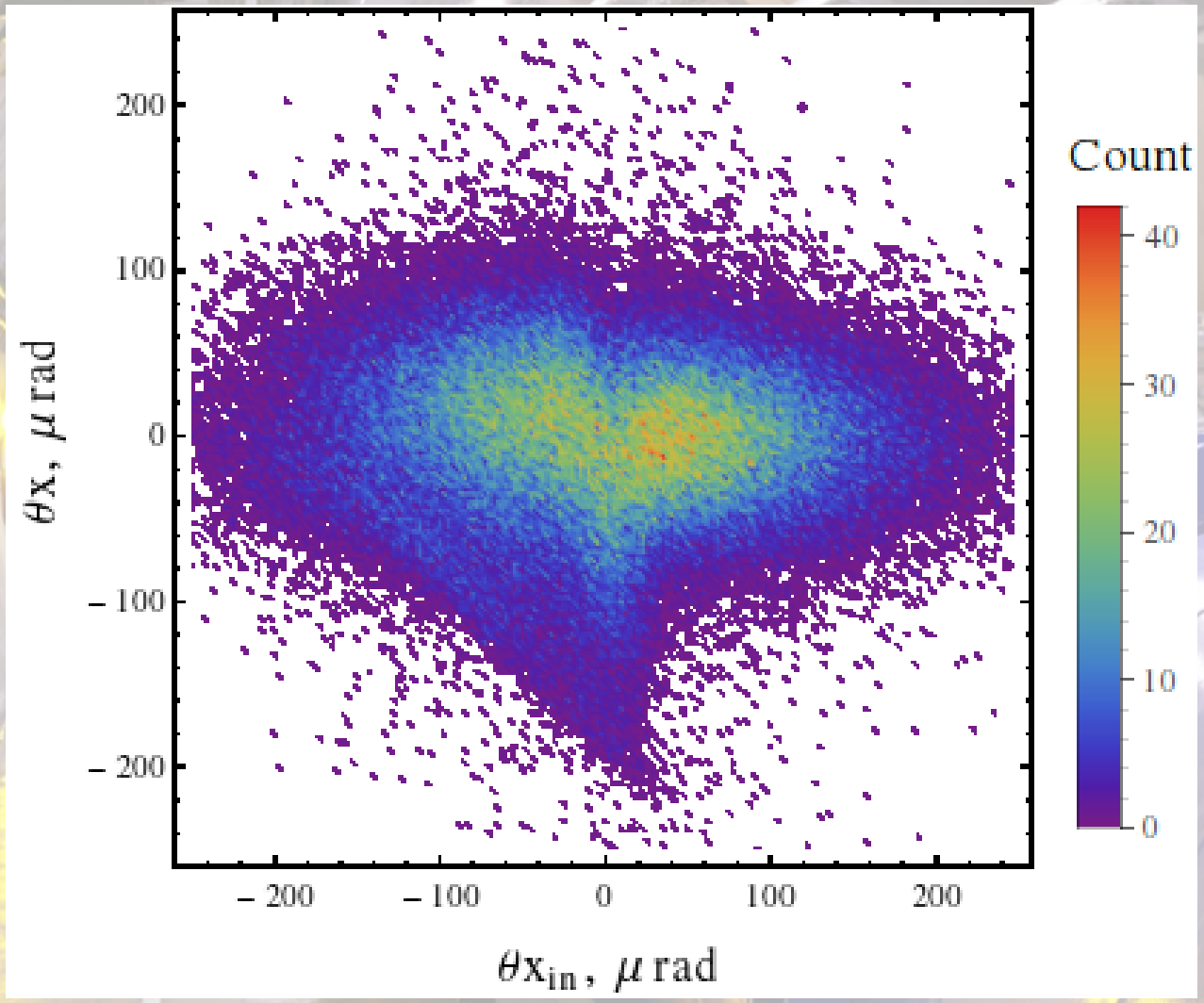

Thank you for attention!

Update of standard physics for Geant4 G4Channeling

New models:
Active only at near channeling conditions (small angles w.r.t. the crystal planes)

- Multiple and single **Coulomb scattering*** on screened atomic potential
- **Single Coulomb scattering on electrons**
- **Ionization energy losses in channeling**

```
void ClAtScattering(G4double &tx, G4double
void ClElScattering(G4double &tx,G4double &
void IonizationLosses(G4double &Ez0,G4doubl
```

```
455 void G4ChannelingS::ClAtScattering(G4double &tx,G4double &ty,G4dou
456 {
457         G4double ksi=0.1;
458
459 //      calculation of the teta2-minimal possible angle of a sing
460         G4double E1=k2*dZEFN; //for high speed of a program
461 //      (real formula is (4*pi*N0*wpl(x)*dz*zz1*zz2*alpha*hdc/ez)
462         G4double teta122=tetamax12/(ksi*tetamax12/E1+1.); // teta
463         G4double teta22;
464         G4double t;
465 //      if the angle of a single scattering is less teta1 - minim
```

The **Coulomb scattering model** in the **CRYSTALRAD** simulation code has been experimentally validated at the Mainzer Mikrotron **MAMI***

Revised Class **G4ChannelingOptrChangeCrossSection (G4VBiasingOperation): turning off** when channeling simulation is active of:

- **Coulomb scattering** processes
- **Ionization energy losses**

The verification of both **Physics Lists** and modification of the cross sections in **G4ChannelingOptrChangeCrossSection** is **in progress**

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