SUMMARY OF EM PARALLEL SESSIONS

S. Guatelli & L. Pandola

on behalf of the EM working group

27th Geant4 Collaboration Meeting, September 30th, 2022

EM parallel session 2A, Sep 27th

New developments for EM physics

Tue 27/09

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09:00	**Recent developments and validation of Geant4 PIXE**	*Susanna Guatelli*	
	TD1	09:00 - 09:20	
	New Geant4 model of channeling in crystals and its potential applications	*Alexei Sytov*	
	TD1	09:20 - 09:40	
	Development of a physics list for radiation protection studies in space	*Jay Archer*	
	TD1	09:40 - 10:00	
10:00	**Development of Geant4-DNA for atmosphere simulations**	*francesca nicolanti et al.*	
	TD1	10:00 - 10:20	

Recent developments and validation of Geant4 PIXE

Contribution by S. Guatelli

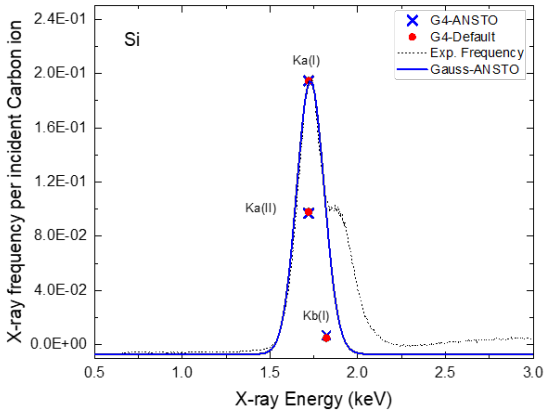
- Describes:
  - PIXE for alpha and proton ionization (cross sections available up to 5 MeV)
  - Fluorescence yields (K, L and M shells)
  - Developed and validated by the Australian ANSTO
- *Alternative* to the models existing in Geant4
  - Available since Geant4 11.0 (G4EMLOW 8.0)
- Validation with protons (2-3 MeV), alphas (10 MeV) and C ions (1-3 MeV/A) on several targets (low-, medium- and high-Z) using **`TestEm5`**, data from ANSTO
  - First validation for **C ions**
  - Tested against the G4 default (ECPSSR Form Factor)
    - Agreement few % for K-shell,10-50% for M- shell
  - Good agreement against ANSTO data
  - Relaxation using the EADL libraries (default) or the custom ANSTO-HP
    - ANSTO gives systematically a higher fluorescence yield

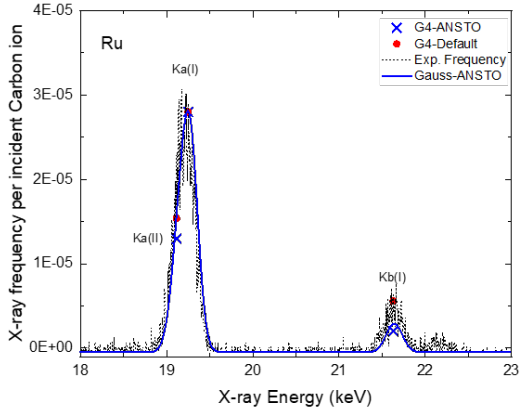
Recent developments and validation of Geant4 PIXE

Contribution by S. Guatelli

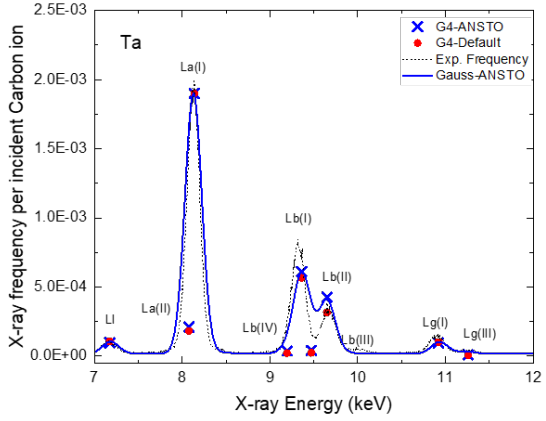
Carbon ions

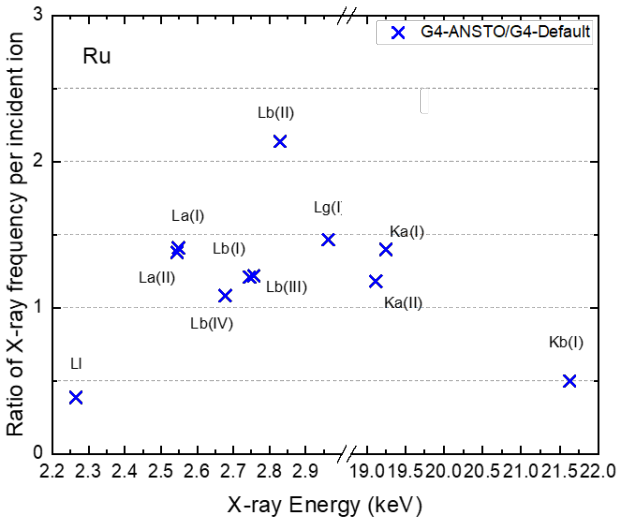
1 MeV/u ^{12}C

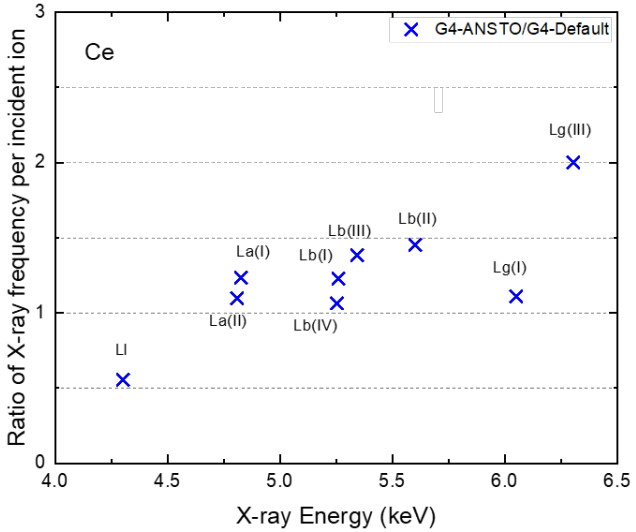


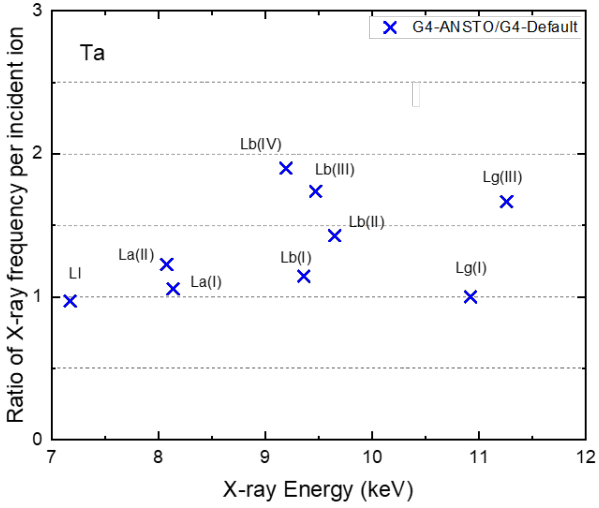


Carbon ions









New Geant4 model of channeling in crystals and its potential applications

- Marie Curie project TRILLION
- New implementation of channeling (trajectory) for charged particles
  - Model from CRYSTALRAD
  - Ready for release
- Makes use of **FastSim interface**
- Radiation model in progress

Contribution by A. Sytov

KiSTi www.kisti.re.kr Korea Institute of Science and Technology Information

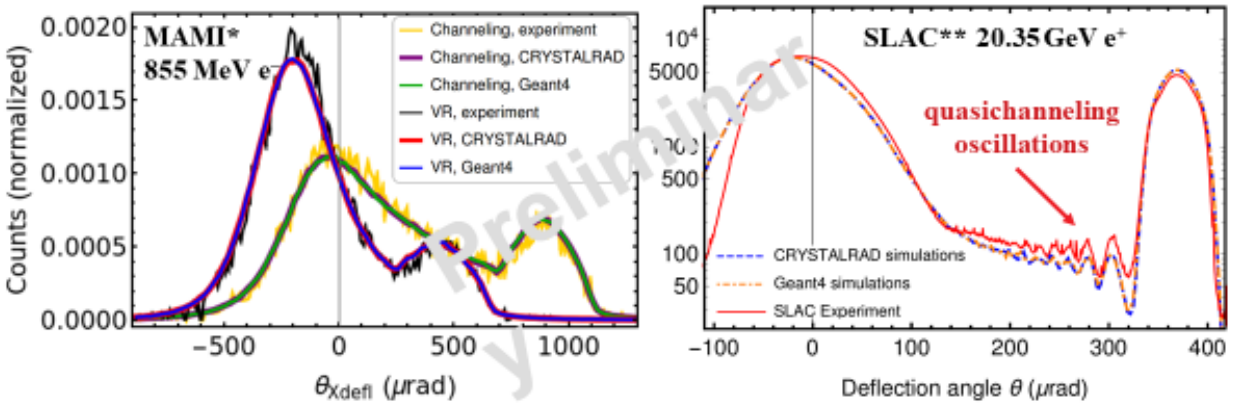
INFN Istituto Nazionale di Fisica Nucleare

European Commission

Trillion

GEANT4 A SIMULATION TOOLKIT

Geant simulations vs experiment and CRYSTALRAD simulations



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

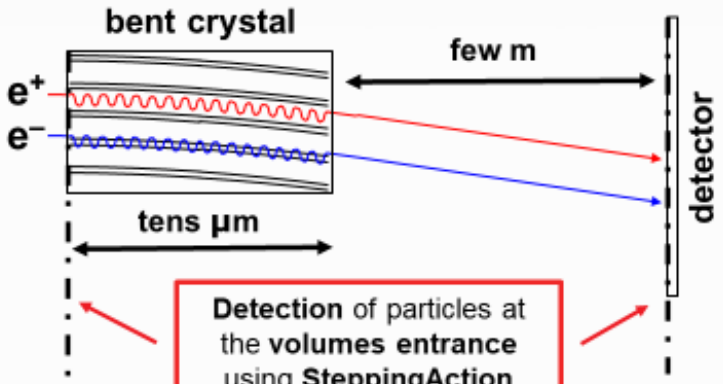
**T. N. Wistisen, ..., and A. Sytov. Phys. Rev. Lett. 119, 024801 (2017)

New Geant4 model of channeling in crystals and its potential applications

- First Geant4 channeling example for e^-/e^+
- Benchmarked against experimental data
- Tested in Seq/MT
  - Ready for release

Contribution by A. Sytov

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 **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

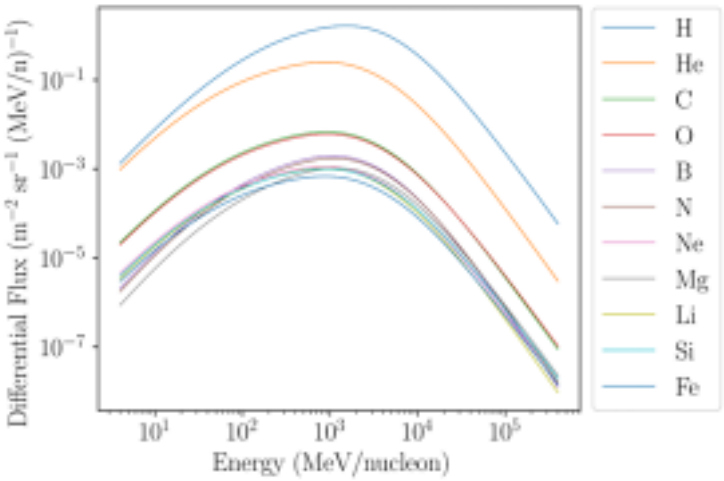
*A. Mazzolari et al. Phys. Rev. Lett. 112, 135503 (2014)

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

Development of a physics list for radiation protection studies in space

Contribution by J. Archer

- Study of the radiation protection issues in lunar environment
  - The radiation environment on the moon consists of primary high energy GCR ions and secondary radiation generated within the lunar volume



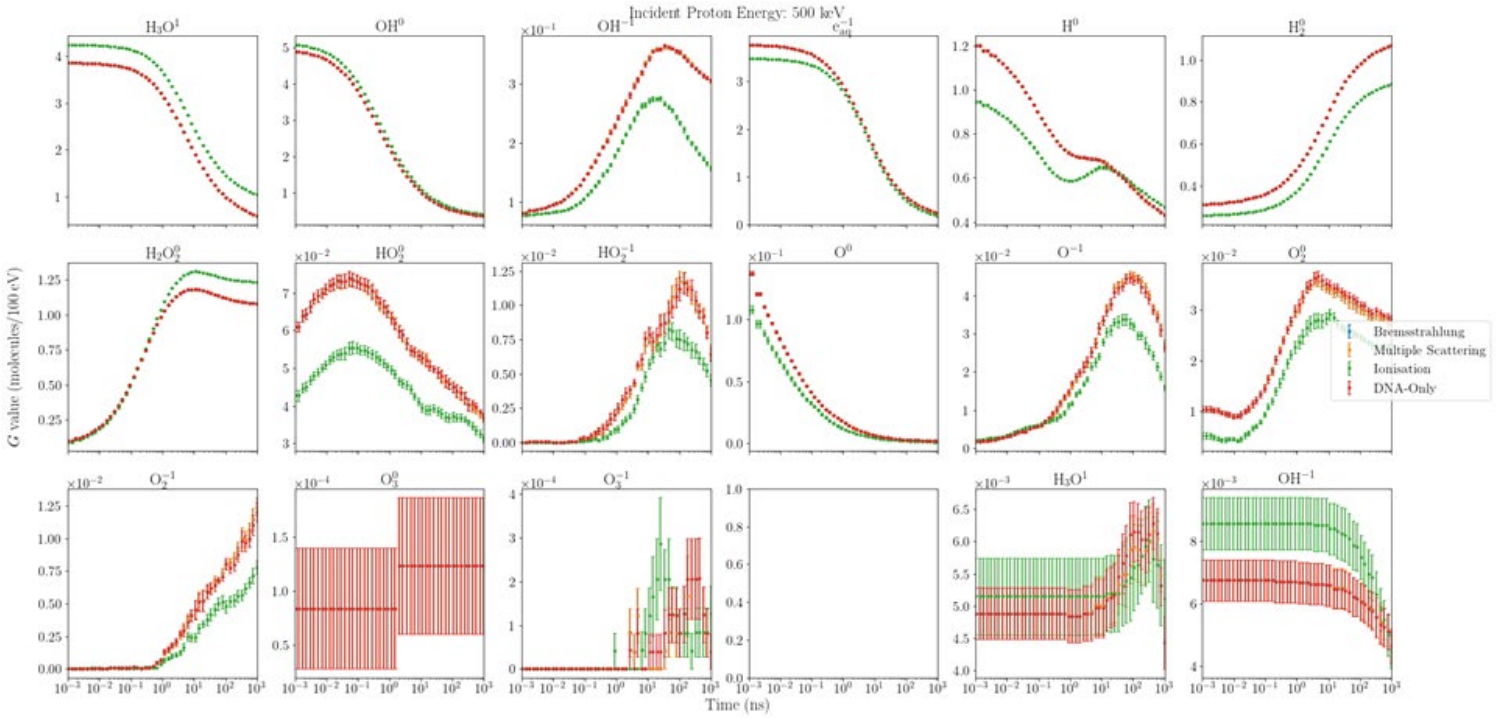
GCR spectrum during solar minimum as modelled using SPENVIS

  - Currently Geant4-DNA models cover a limited energy range for space applications:
    - Protons/ions: up to 100 MeV
    - Electrons: up to 1 MeV
  - Thus, a hybrid Geant4 and Geant4-DNA physics is desired for space applications

Development of a physics list for radiation protection studies in space

Contribution by J. Archer

- **Problem** found with radiochemical yield (**`chem6`**)
  - Radiochemical yields observed to vary between hybrid and pure-DNA, even when the simulation is entirely in the DNA energy range
  - Somewhat related to electron ionisation
    - Stopping power invariant and no differences in process activation apparent



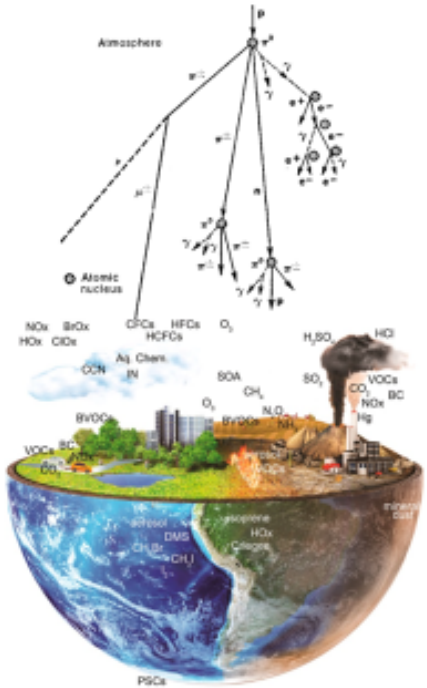
Development of Geant4-DNA for atmosphere simulations

Contribution by F. Nicolanti

- First application of Geant4-DNA to environmental physics

Geant4DNA for atmosphere

PhD student: F. Nicolanti, Thesis Advisor: Dr. C.M. Terracciano,
External Advisor: Dr. B. Caccia



Motivation:
The way cosmic rays and ions can alter the balance of important molecules is a still poorly studied aspect in the atmospheric models.

The AIM:

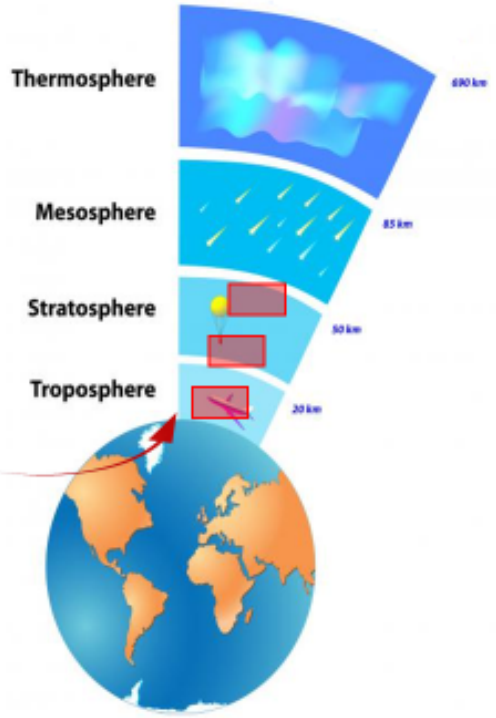
Accurately describe the **amount and state of ionisation, and the spatial distribution of ions produced by CR** interaction in small volumes at different altitudes in the atmosphere.

The HOW:

By **including in Geant4-DNA models** for particle-impact interactions with relevant molecules for climatology

The Starting point:

e- impact interaction on N2 and O2: Ionisation, Elastic scattering, Electronic excitation.



External Collaborators: **A. Cartoni, M. Satta** (Sapienza Chemistry, Rome), **S.Incerti, H.N. Tran** (CNRS / IN2P3, France), **D. Emfietzoglou, I. Kyriakou** (Ioannina, Greece).

Development of Geant4-DNA for atmosphere simulations

Contribution by F. Nicolanti

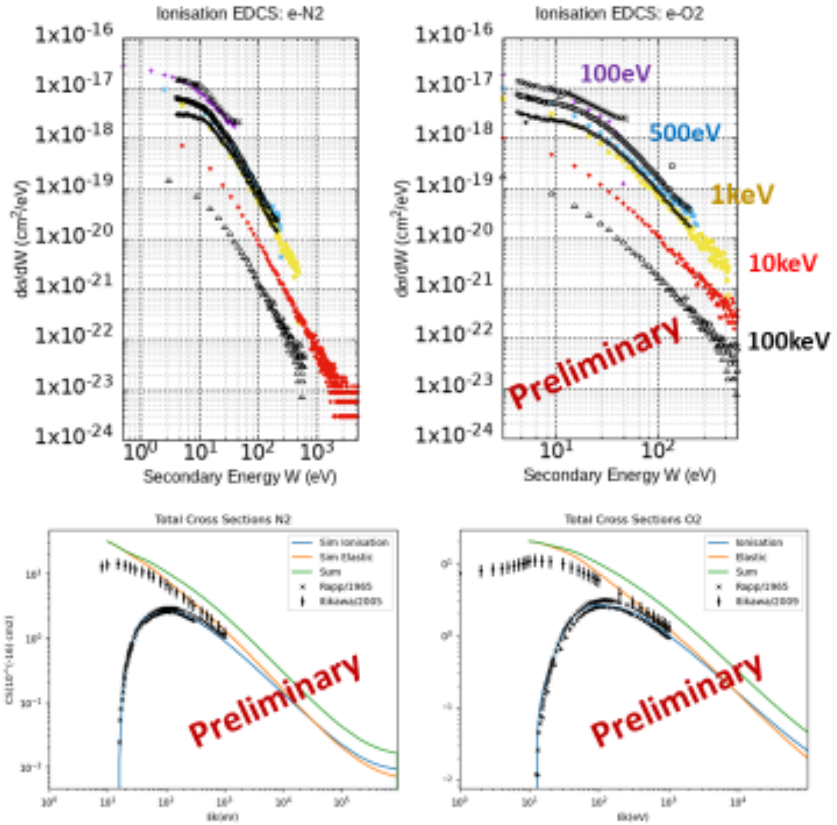
- Model of e^- impact interaction with N_2 and O_2 in Geant4-DNA

What has been implemented:

- Ionisation Total and DCS – RBEB model
  - **Energy range:** threshold - 1GeV
  - **Type**: analytical
  - N2: 4 outer-shell, O2: 5 outer-shells
- Elastic scattering Total and DCS - ELSEPA code
  - **Energy range:** 100 eV - 1GeV
  - **Type**: interpolated CS data tables

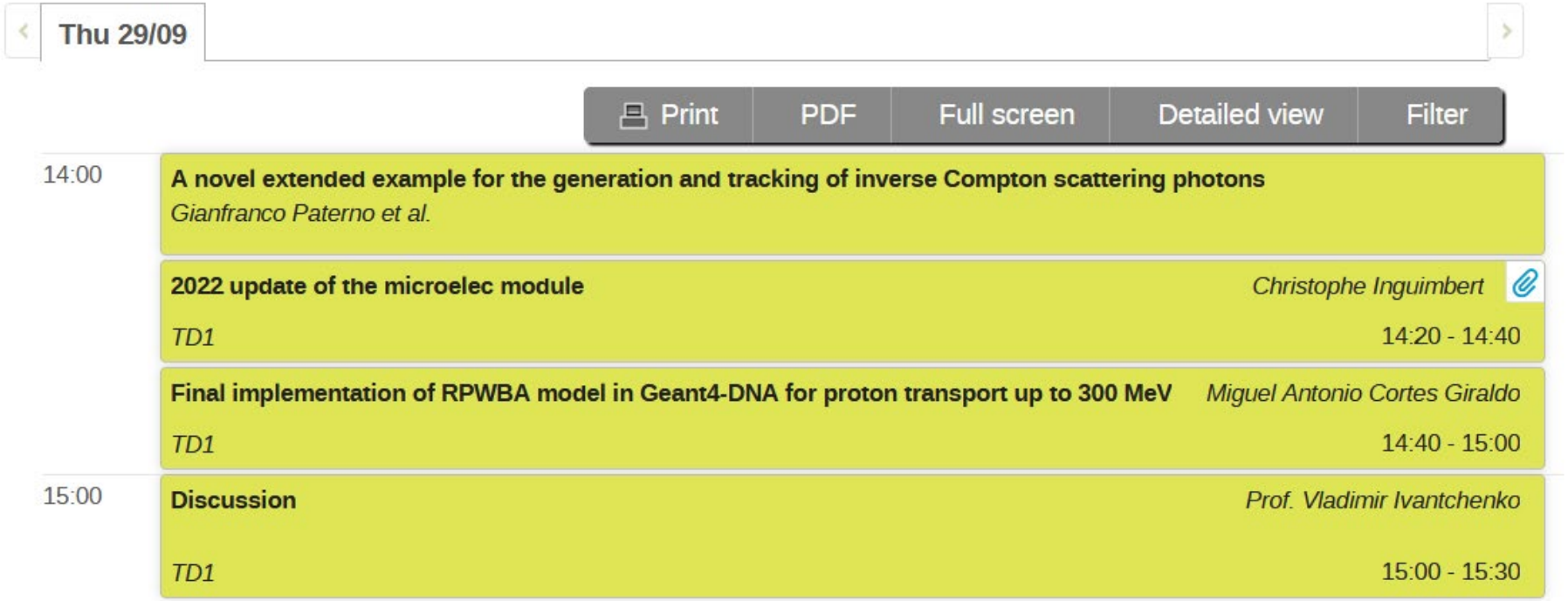
WORK in PROGRESS:

- Ionisation: Inclusion of inner N,O k-shells
- Elastic scattering:
  - complement the model with weighted average of exp data for E< 100eV;
  - Systematic study to find the best empirical parameters of the optical interaction potential
- Find the best electronic excitation model:
  - Bef-scaling, R-matrix, exp data, …



EM parallel session 5A, Sep 29th

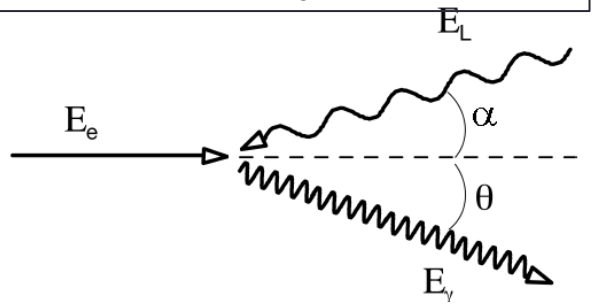
New results for EM physics



Proposal of a novel extended example for the generation and tracking of inverse Compton scattering photons

- The inverse Compton scattering is implemented as a *primary particle source* (not as a process)
  - e^- beam on "eV-photons" target
- The particle generator can be chosen between 5 different options:
  1) read the phase-space from a text file
  2) read the phase-space from a root file
  3) sampling from an ICS parametrization
  4) GPS
  5) exact LCS generation (phase-space saved)
- The phantom is conceived for studies of medical imaging
- Geometry and Source can be set through macros
  - The user can track ICS photons in a simple setup with slits, phantom and detector
- Use a primary generator here, but **physics content**! → move to kernel?

Contribution by G. Paternò



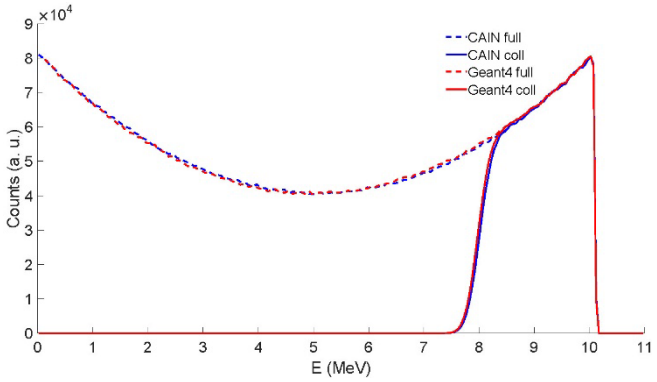

```
/lcsgs/ebeam/energy 43.3e6   #mean energy (eV)
/lcsgs/ebeam/espread 2.e-3   #relative spread (sigma)
/lcsgs/ebeam/emitx 1.5e-6    #x norm. emitt. (m*rad)
/lcsgs/ebeam/emity 1.5e-6    #y norm. emitt. (m*rad)
/lcsgs/ebeam/alphax 0.0015   #Twiss parameters
/lcsgs/ebeam/alphay 0.0021
/lcsgs/ebeam/betax 0.00814   #(m)
/lcsgs/ebeam/betay 0.00814   #(m)
/lcsgs/ebeam/sigmaz 4.e-4 m  #bunch length
/lcsgs/laser/wavelength 1.03e-6  #m
/lcsgs/laser/Zrx 0.01098         #x Rayleigh length (m)
/lcsgs/laser/Zry 0.01098         #y Rayleigh length (m)
/lcsgs/laser/sigmaz 6.e-4 m      #pulse length
/lcsgs/laser/polphi 0.5      #in units of PI (0->x, 0.5->y)
/lcsgs/laser/poldeg 1            #polarization degree
/lcsgs/collAngle 7               #collision angle (deg)
/lcsgs/collRate 1.               #collision rate (Hz)
/lcsgs/eBunchCharge 400.e-12  #(C)
/lcsgs/laserPulseE 0.01          #(J)
/lcsgs/solidangle 50.e-3         #thetamax (rad)
/lcsgs/position 0 0 0 cm
/lcsgs/zlim1 -0.01 m
/lcsgs/zlim2 0.01 m
/lcsgs/zcut 0.01
/lcsgs/list

/run/printProgress 100000
/run/beamOn 1000000
```

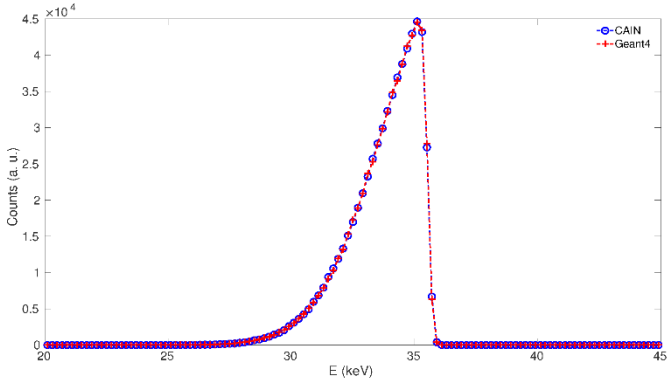
Proposal of a novel extended example for the generation and tracking of inverse Compton scattering photon

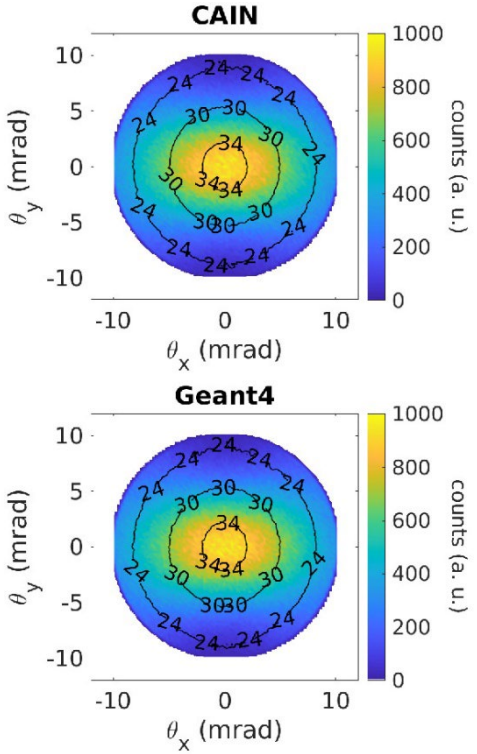
Validation of the developed code: comparison with CAIN

- 3 different cases considered (**BriXS**, NewSUBARU, ELI-NP-GBS)
- Excellent agreement in general, slight differences only for high energy collimated beams and in the spatial distribution at IP (larger spots in CAIN)
- 200 time faster than CAIN

Contribution by G. Paternò



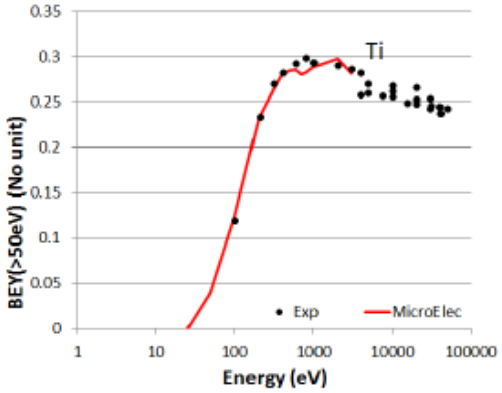


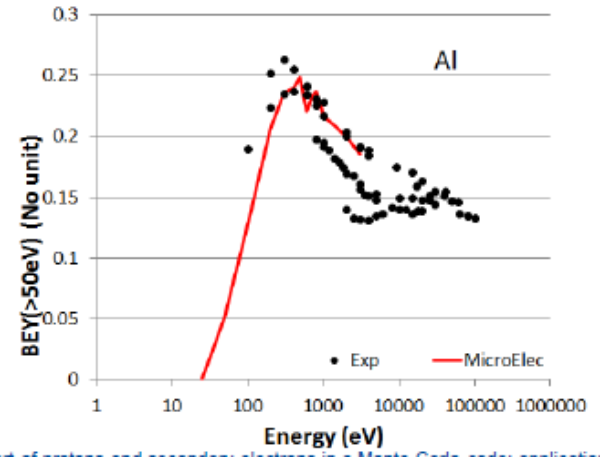


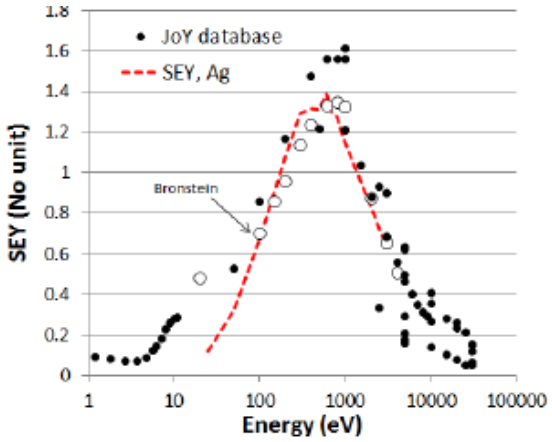
Geant4 MicroElec Module 2022 update

Contribution by C. Inguimbert

- Validation against experimental measurements in terms of Secondary Emission Yield







- **Revisions:**
  - Weakly bound electrons are treated like core electrons
  - The non-ionizing deposited energy is accounted by means of Lindhard energy partition

Geant4 MicroElec Module 2022 update

Contribution by C. Inguimbert

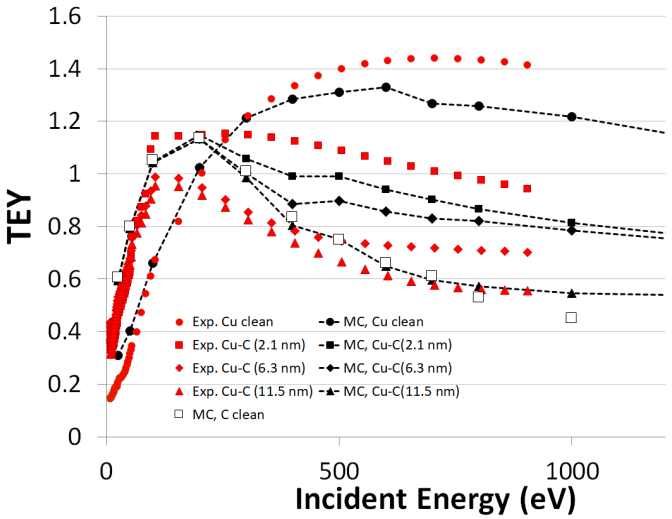
Crosssection database for incident electrons

Database recalculated for the full list of materials

Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, Au, W
Kapton, SiO2, Al2O3, TiN, BN

Eroneous data below the low limit energy have been removed
File size devided in average by a factor ~ 5

REGRESSION TESTS for the full list of materials (SEY metric)



- The advanced example **`MicroElec`** will show how to use the novel cross sections
- Validation against experimental measurements:
  - Inguimbert et al (2022) NIMB 526,1

In the future :

- Extending the material database (GaAs, GaN, CuO, Cu2O, TiO2, MgO, …)
- Providing new examples
  - Calculation of the dose depth profile for low energy electrons and protons
- Below the energy needed to excite a plasmon (~ some tens of eV) **BINARY collisions** becomes the main interaction process. A binary collision model has been implemented in order to replace interaction cross sections for incident protons.

"Use of combined linear and nonlinear formalisms applied to the transport of protons and secondary electrons in a Monte-Carlo code: applications for space missions"
P. Caron, C. Inguimbert, Q. Gibaru, M. Pinson
JAP 2022 accepted

- Cross sections must be recalculated for heavy particles protons and ions following **BINARY** approach (+ regression test)

Final implementation of RPWBA model in Geant4-DNA for proton transport up to 300 MeV

http://geant4-dna.in2p3.fr/

Max. energy Limit → 100 MeV

Max. energy of clinical proton therapy beams → ≈250 MeV

Range in liquid water → ≈ 39 cm

Contribution by M. A. Cortés-Giraldo

PROTONS (named "proton") — Liquid water

- **Nuclear scattering** : G4DNAElastic
  - G4DNAIonElasticModel
    - applicable energy range : 100 eV - 1 MeV
    - cut at 100 eV (5)
    - type : interpolated
    - Geant4-DNA physics constructors : default, option2, option4, option6
- **Electronic excitation** : G4DNAExcitation
  - G4DNAMillerGreenExcitationModel
    - applicable energy range : 10 eV - 500 keV
    - type : analytical
    - constructors : default, option2, option4, option6
  - G4DNABornExcitationModel (3)
    - applicable energy range : 500 keV - 100 MeV
    - type : interpolated
    - constructors : default, option2, option4, option6
- **Ionisation** G4DNAIonisation
  - G4DNARuddIonisationModel (G4DNARuddIonisationExtendedModel is also usable, °)
    - applicable energy range : 0 eV - 500 keV
    - cut at 100 eV (5)
    - type : interpolated
    - constructors : default, option2 (°), option4, option6
  - G4DNABornIonisationModel
    - applicable energy range : 500 keV - 100 MeV
    - type : interpolated
    - constructors : default, option2, option4, option6
- **Electron capture** : G4DNAChargeDecrease
  - G4DNADingfelderChargeDecreaseModel
    - applicable energy range : 100 eV - 100 MeV
    - type : analytical
    - constructors : default, option2, option4, option6

Increase these limits!

G4DNARPWBAExcitationModel.cc
G4DNARPWBAIonisationModel.cc

Models

G4DNAExcitation.cc
G4DNAIonisation.cc

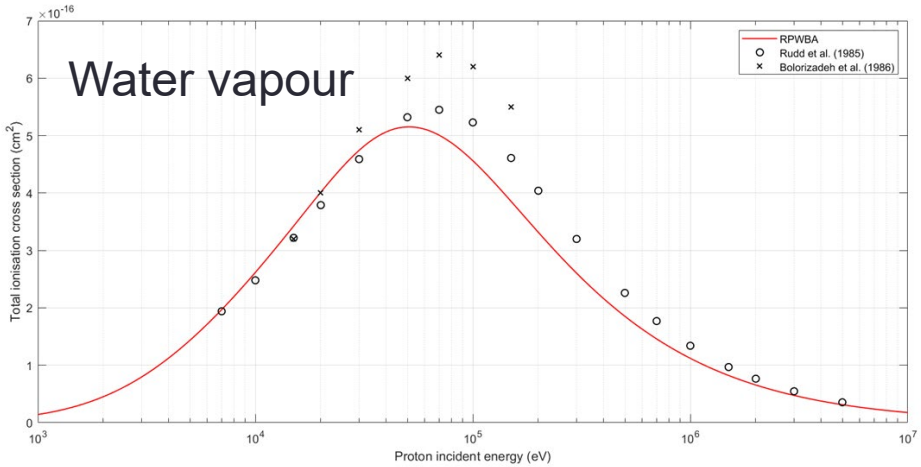
Processes

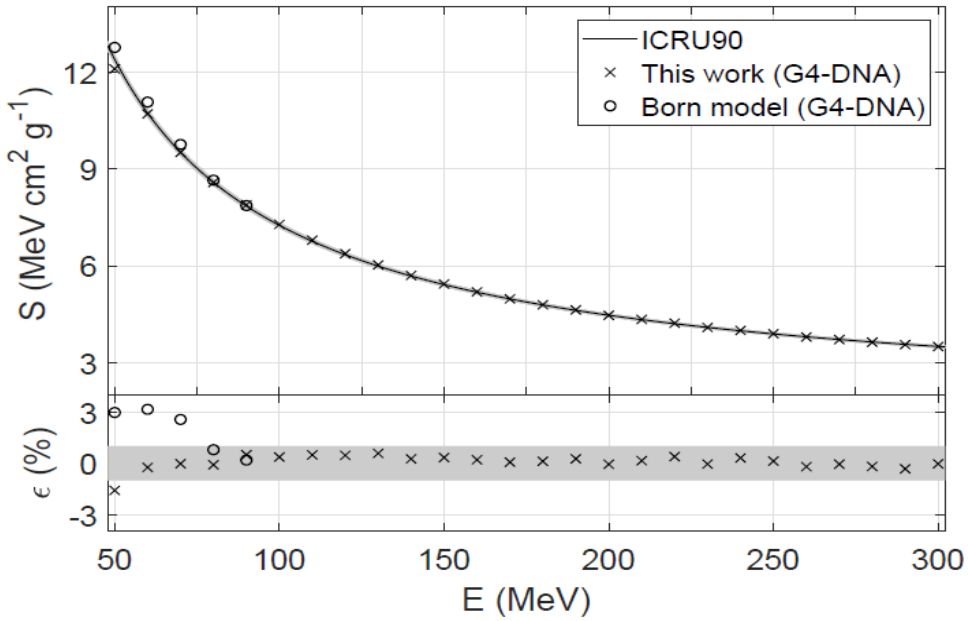
- New RPWBA processes and models available on **`gitlab`**
- Implementation analogous to **`G4DNABorn`** models

Benchmarking

Contribution by M. A. Cortés-Giraldo

- New G4DNA model available for protons up to 300 MeV
- Maximum deviation w.r.t. existing Born model of 5% and 2%, ionization and excitation, respectively, for protons at 100 MeV
- Agreement with ICRU90 values:
  - **`spower`**: within 1%.
  - **`range`**: within 0.5% for proton stopping above 100 MeV
- Work documented in
  - D. Domínguez-Muñoz et al., Radiat. Phys. Chem 199: 110363 (2022)





Discussion on EM Physics problems

Contribution by V. Ivantchenko

- Implementation of EPICS2017 for Livermore photon models completed
- Bug reports which will be **closed** within Geant4 11.01
  - 2510 (D. Sawkey) boundary reallocation step doesn't happen
  - 2495 (V. Ivantchenko) Problem dEdx and ranges for low-energy ions
  - 2494 (V. Ivantchenko) RadioactiveDecay process do not work with emstandard_opt0 or local physics list
  - 2475 (P. Cirrone) Phantom data files are incorrectly read in from file (Responsible to be changed to S. Guatelli)
  - 2452 (V. Ivantchenko) SIGFPE issue in G4VRestDiscreteProcess
  - 2412 (V. Ivantchenko) DNA physics deactivates radioactive decay physics
  - 2354 (V. Ivantchenko) Segmentation fault caused when processes are disabled via the user interface
  - 2279 (V. Ivantchenko) problem with dexcitationIgnoreCut
  - 2235 (H. Tran) G4Track returns incorrect coordinates and step lengths of chemical species

Pending tasks/problems

Contribution by V. Ivantchenko

- Improve coverage of validation and "early warning" system
  - Ask to run all tests (EM, G4-Med, etc) on geant-val for Geant4 11.0.08
  - Liaise with D. Konstantinov
- Double check if Bragg peak and ion range is fine or damaged before the release (M. A. Cortés-Giraldo)
- Problems connected with the combination of EM Standard/ Geant4-DNA physics lists should be solved (→ Jay Archer talk)
- Technical problems in `MicroElec` models should be solved (→ Coverity analysis)
- Development of a coherent approach and effort to perform regular benchmarking activity: in progress