Geant4 updates : EM Physics and Fast Simulation

15th Geant4 Space Users' Workshop,

5th – 7th December 2023,

Hyatt Place Pasadena,

Marc Verderi (LLR)

Introduction

- **Electromagnetic part:**
  - Many things happened since last Space Users' Workshop
    - We may mention:
      - **Creation of a new library : G4HepEM, by Mihaly Novak (CERN)**
        - Separating (heavy) initialization code –to perform the many calculations- from (light) one at run time –just fetching a few numbers-
      - **G4GammaGeneraProcess**
        - A super process that encapsulates all gamma physics
        - Brings some performances boost (~5%)
        - But allows using option like Wookcock tracking
      - **G4TransportationWithMSC**
        - Merge of transportation and multiple scattering
        - Main motivation is performances, as allowing many back and forth calculations between the two, without going through the stepping manager
  - Many recent activities in the EM ("standard EM") consist in code consolidation and improvements
    - Code cleaning, rationalizing, etc.
    - Consolidation like for example tackling some fragilities introduced with ICRU90
    - I will not detail
  - The low energy EM, and in particular DNA, has many recent developments
  - In this presentation, I will focus on recent developments, in particular those most related to space

- **Fast Simulation part:**
  - A shorter part, but with promising features, very Machine-Learning focuses

Developments in EM Domain

Standard and DNA

X-Ray reflection process

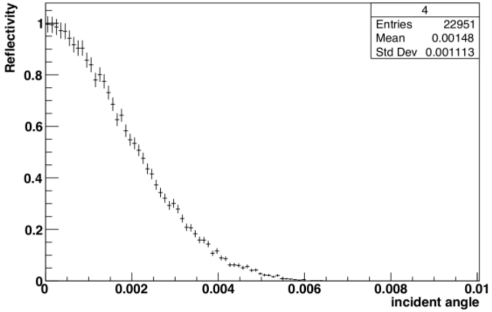
Helmut Burkhardt (CERN)

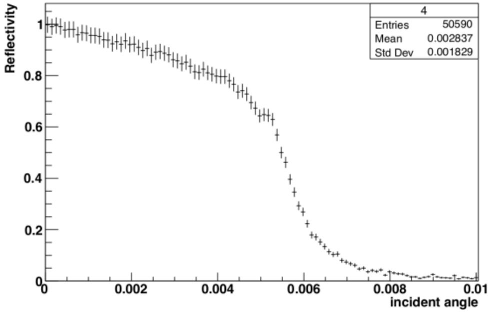
- **Useful for space application, for X-ray telescopes…**
- … **but author, from HEP, had a different initial motivation:**
  - *It came as a (bad) surprise in LEP : hard (5-10 keV) X-ray photons from synchrotron radiation generated in magnets as far as 200 m from the interaction region can undergo specular (mirror) reflection on the vacuum chamber and reach the interaction region and strongly enhance detector backgrounds.*
  - G.v. Holtey, et al., NIM A403, 1998
  - **Strong motivation** : FCC-ee studies, with in particular FCC-MDI

- **Main reference considered:**
  - B.L. **Henke**, E.M. Gullikson, and J.C. Davis. *X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30000 eV, Z=1-92*, Atomic Data and Nuclear Data Tables Vol. 54 (no.2), 181-342 (July 1993)
  - Used to compute the **real and imaginary parts of reflective index**.
  - Re-use existing components / tools in Geant4 for the concrete implementation

- Development illustrated in new TestEm16 example (September)
- **Development is part of 11.2 .**

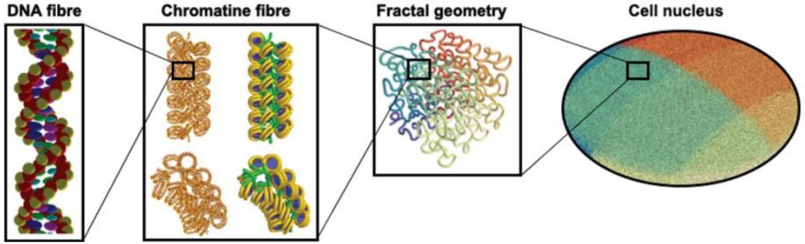
Preliminary tests from TestEm16 : scan in angle for two mean angles



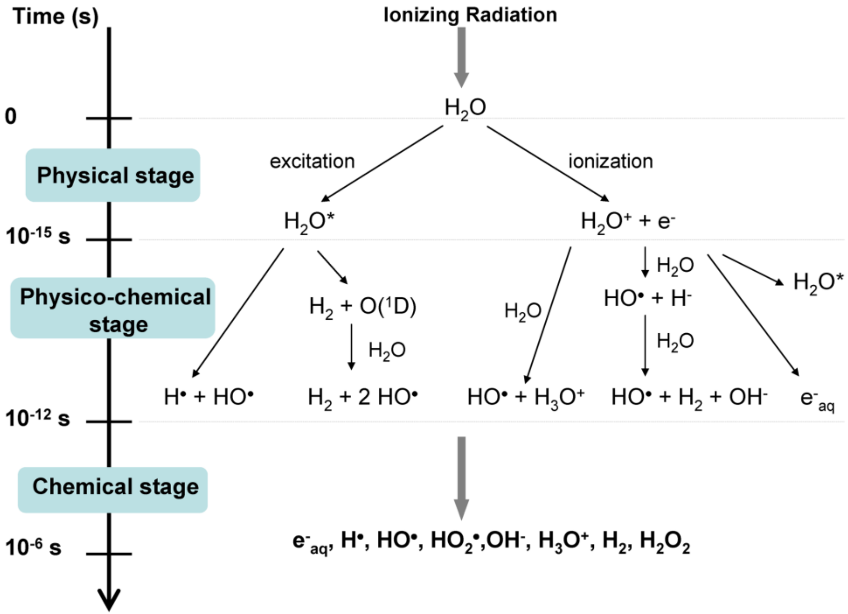


DNA approach reminder

- Bottom-up approach of the dose

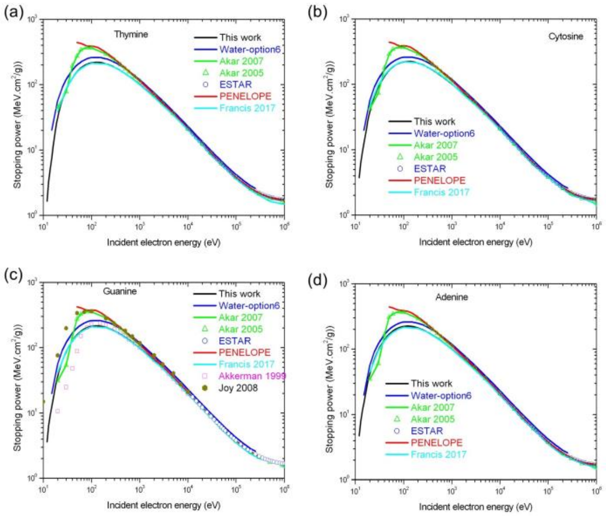


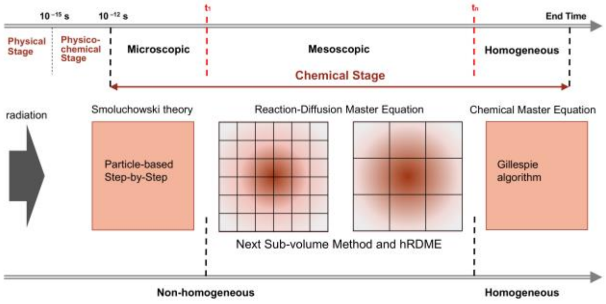
- Initiated by ESA for manned mission to Mars
- Proceeds as:
  - Tracking phase :
    - With no “condensed history” applied
      - All individual interactions are calculated
    - Down to O(eV) for some interactions
  - Chemistery phase :
    - Diffusion of radical species, with mutual interaction
  - Both phases contribute to damages to DNA
    - ~40% + ~60% respectively
- Initially considering liquid water as tracking medium
  - More materials being added over time
    - Note : these are “particle – molecule” interactions
- **Approach also applied to silicon, with MuElec**
  - Aluminium oxide, Boron nitride, and Silicon dioxide are now available in addition to the initial Silicon.



G4-DNA recent developments

- **Improved electron transport in liquid water 10 eV – 10 MeV**
  - Various aspects, leading to more radiotherapy applications
  - Implemented in DNA_Option4 model
- **Extend the tracking of protons from 100 MeV to 300 MeV**
  - Intended for medical application (100 MeV ~ 7 cm range in water)
  - Keeping the G4-DNA proton – medium interaction details
    - 5 ionized molecular states, 5 excited molecular states and electron capture
  - Treatment based on:
    - Projectile : Relativistic Plane Wave Born Approximation (RPWBA)
    - Target response : Generalized Oscillator Strength (GOS)
- **Extend target material set:**
  - All DNA materials (Adenine, Guanine, Thymine, Cytosine, Deoxyribose, Phosphoric acid)
    - Elastic scattering (Independent Atomic Model), Ionisation (Relativistic Binary Encounter Bethe Model), Excitation (scaled from water inelastic XS and bases ionisation XS)
    - Energy range (11 eV – 1 MeV)
  - O_2 and N_2 (see after)
- **Chemical stage:**
  - Develop a "mesoscopic" approach to deal with diffusion times > 1 μs
- **New geometries:**
  - Used in moleculardna, dnadamage2 and dsbandrepair examples





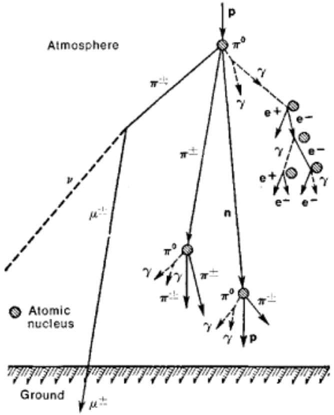
G4-DNA… in atmosphere

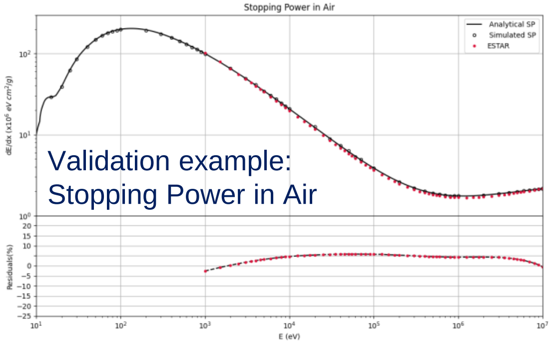
F. Nicolanti (INFN) *et al.*

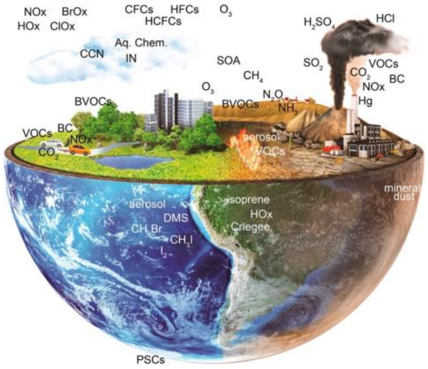
- **Ions formed in the atmosphere by cosmic rays may have a strong impact on its composition:**
  - They may dramatically change chemical reaction rates (up to 10 order of magnitudes !)
  - Studies suggest their role in precipitation, cloud cover, nucleation, ozone depletion, aerosol formation…
- Ion formation already simulated, but with condensed history, "not very low" energy processes, no molecular description

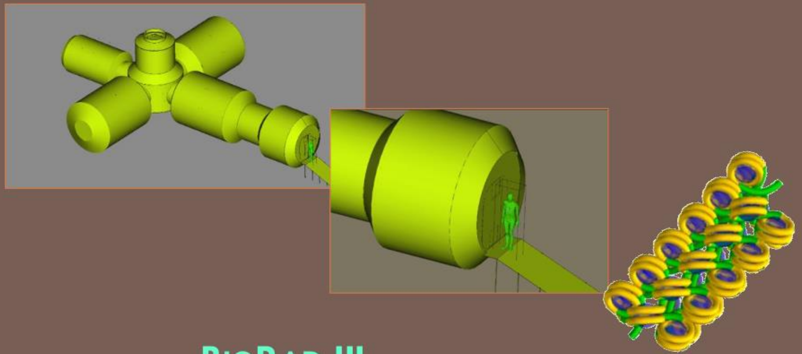
- **This motivates the development of a G4-DNA-like study**

- **Goal is to obtain:**
  - Ionic density, state of ionization, spatial (altitude) distribution of ions, chemical species produced
- **Starts with precise $e^{-} - O_2$ or N_2 interactions**
  - Gaseous phase, molecular description
  - Ionisation, elastic scattering, electronic excitation (**)
  - Energy range 10eV – 10 MeV
- **Status:**
  - Cross-sections included and validated
  - As well as final state generation
  - Used in models G4AtmXXXModel, XXX = (**)
- **Next step: perform first simulations by importing cosmic rays spectra at different altitudes (5 - 25km)**









BioRad III

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BioRad III at a glance (2)

3

- A consortium of 9 EU partners
  - Full contract **ESA with Centre National de la Recherche Scientifique** (CNRS, France)
    - 400 k€, 2 years (2021-2023)
  - Sub-contact **CNRS with subcontractors**
    - Centre Hospitalier Universitaire Vaudois (Switzerland)
    - Commissariat à l'Énergie Atomique et aux énergies alternatives (CEA, France)
    - G4AI Ltd (UK)
    - National Institute for Nuclear Physics (INFN, Italy)
    - Institut de Radioprotection et de Sûreté Nucléaire (IRSN, France)
    - SWHARD SRL (Italy)
    - University of Ioannina (Greece)
    - University of Sevilla (Spain)
  - Including **external collaborators**: Belgrade U., Serbia; JINR, Russia; Osaka U., Japan; Wollongong U., Australia

BioRad III at a glance

2

- Objective
  - **Open multi-scale radiation effects platform for radiation protection in space**
    - Simulate the effects of ionizing radiation on biological matter
      - Radiation physics : particle- matter interactions in « discrete » mode
      - Radiation chemistry : production of molecular species, diffusion, chemical reactions
      - Radiation biology : early DNA dame induction and repair
    - In a multi-scale environment
      - From space habitats to realistic human phantoms and biological cells
  - No equivalent software currently accessible to the scientific community
  - Open source approach
    - Based on the open-source simulation tools Geant4/Geant4-DNA and GRAS, strongly supported by ESA

Conclusion

23

- BioRad III has allowed the development of key functionalities in the Geant4, Geant4-DNA and GRAS tools
  - Allowing in particular the development of a prototype multi-scale simulation platform based on the FreeCAD framework
  - Key components : DNA-scale chain & geometries, MINAS-TIRITH, phantoms, space habitats
- Such a platform can be used in the context of space missions, combining detailed geometries of space habitats and realistic human phantoms, down to the cellular scale
- Dedicated experiments have been performed to verify/validate recently released software for radiolysis simulations, and for radiobiological simulations based on the Geant4 and Geant4-DNA tools
- Described software is being/will be included in Geant4 and/or GRAS
- The creation of a common radiobiological database, in particular for the validation of radiobiology simulations, will probably be useful for the scientific community

Thank you !

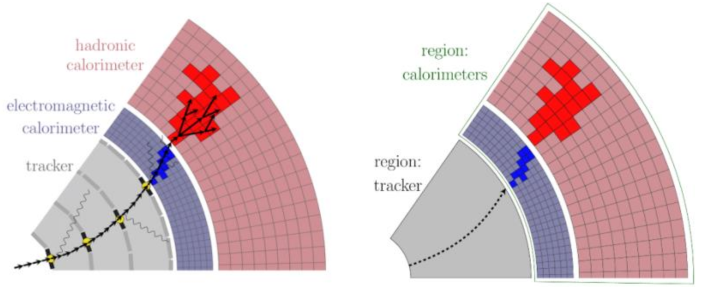
Fast Simulation

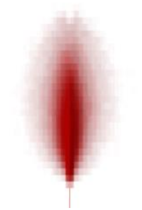
Fast Simulation Progress

Anna Zaborowska, Dalila Salamani (CERN)

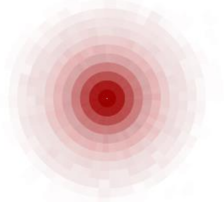
- **What is “fast simulation” ? (FS)**
  - In HEP “fast simulation” classically refers to “fast shower simulation”
  - And is even more restricted in practice to “fast electromagnetic shower simulation” (FS of hadronic showers are rare [1]).
- FS replaces the detailed tracking with an approximate model of energy deposition in the calorimeter(s)
  - Model is in general detector dependent [2]

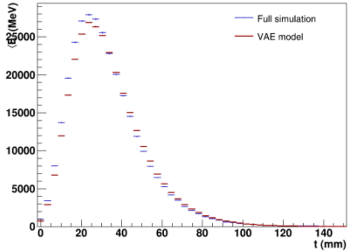
- **On-going work in Geant4:**
  - Investigate usage of Machine-Learning (ML) techniques in replacement of the classical analytical & detector-specific models
    - It may happen that ML techniques resolve [1] & [2] !
  - Focus on electromagnetic showers for now
  - **Exploit Variational AutoEncoder (VAE) model**
    - Used by ChatGPT, DALL-E, …
    - A neural-network with probabilistic connections → naturally varies the generation, request after request
- **Aggregates quite intense activities with LHC experiments !**
  - Eg : Calo Challenge Workshop, 30-31 May 2023 in Frascati

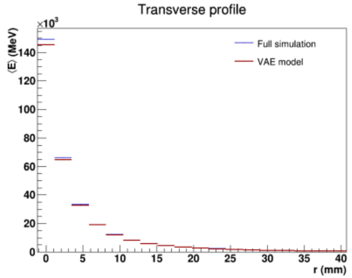




Longitudinal & lateral VAE generated shower profiles

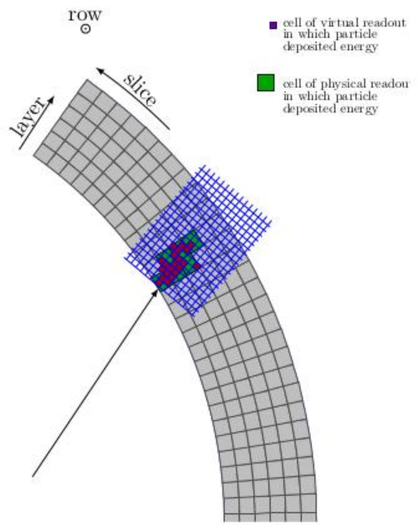




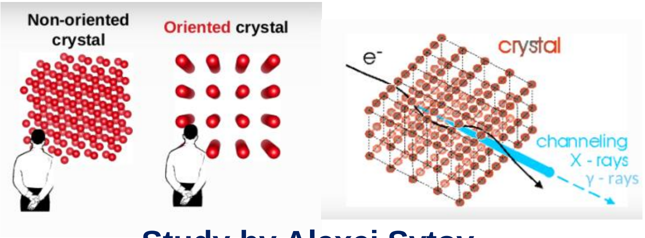


Geant4 example Par04

- **A new example (Anna + Dalila), demonstrates how to build a shower model using ML:**
  - Extended example Par04 shows how to use Machine Learning (ML) models within GEANT4.
  - Distributed with a Variational AutoEncoder (VAE) model of showers used in fast simulation.
  - Demonstrates how to incorporate inference libraries: ONNX runtime, pyTorch, lwtnn.
  - Ability to run it on GPU (a choice done by UI command).
  - It scores energy along shower axis, performs validation of shower observables.
  - Recent additions of physical detector readout for performance benchmarking.



- Note : example **Par04 is not limited to showers**
  - For example, will be used to speed-up tracking in channeling process (not discussed today)



Study by Alexei Sytov

Conclusion

- EM Physics:
  - Standard EM physics package went for quite consolidation this year
  - Still active developments in DNA
  - Many topics are relevant to space domain

- Fast Simulation is exploring Machine Learning usage
  - Which looks promising

- BTW & not much discussed here, but Machine Learning usage is being expanded beyond Fast Simulation