Geant4DNA introduction

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Alberto Sciuto

A lot of material from S. Incerti

Outlook

- Why Geant4DNA?
- Brief History
- Simulation steps
- Examples

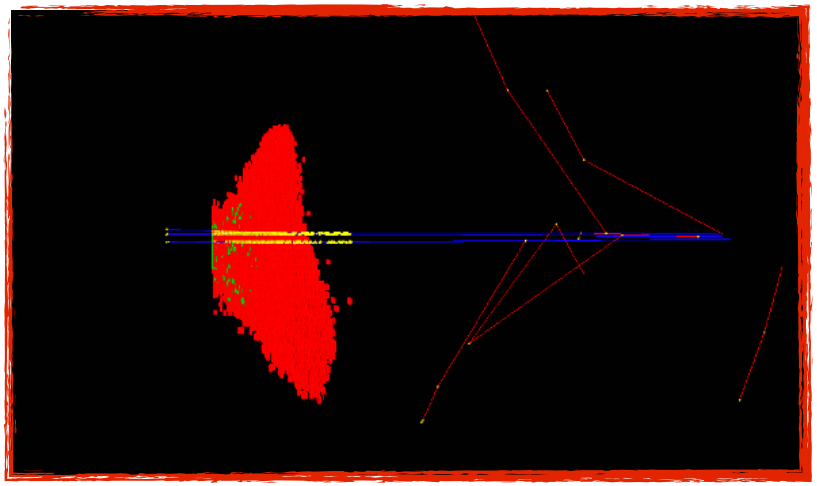
Another Geant4?

Yes, deal with it

- Can we try to extend Geant4 to model biological effects of radiation ?
- Limitations prevent its usage for the modelling of biological effects of ionising radiation at the sub-cellular & DNA scale
  - Condensed-history approach
    - No step-by-step transport on small distances, a key requirement for micro/nano-dosimetry
  - Low-energy limit applicability of EM physics models is limited
    - Livermore Low Energy EM models can technically go down to 10 eV but accuracy limited
    - 100 eV for Penelope 2008 Low Energy EM models
  - No description of target molecular properties
    - Liquid water, DNA nucleotides, other
  - Only physical particle-matter interactions
    - At the cellular level, physical interactions are NOT the dominant processes for DNA damage at low LET...

A brief history of G4 DNA

- 2001 Initiated at the European Space Agency/ESTEC by Petteri Nieminen
- 2007 First prototypes of physics models for liquid water added to Geant4 9.1
- 2008 Development coordinated by CNRS/ IN2P3 (physics, chemistry, geometries)
- 2014 Chemistry stage extension ready for end users in Geant4 10.1

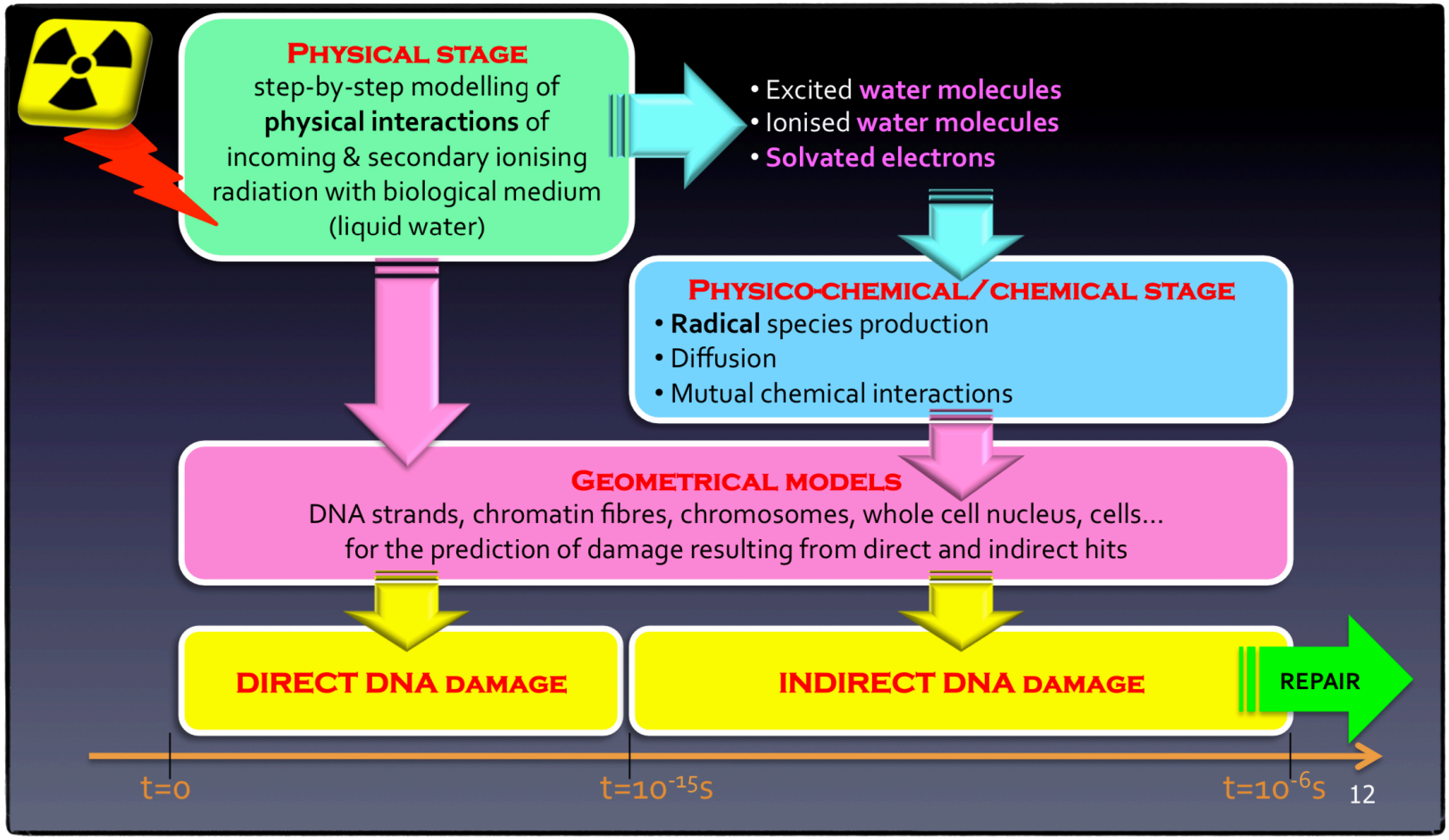


LP2iB-CENBG microbeam irradiation of a keratinocyte with alpha particles from the « microbeam » Geant4 advanced example - movie courtesy of L. Garnier (CNRS) -

Overview of Geant4DNA

- The code is fully included in Geant4
- It is an independent sub-category of the electromagnetic physics category of Geant4: $G4INSTALL/source/processes/electromagnetic/dna
- An interdisciplinary activity of the Geant « low energy electromagnetic physics » working group
- Both are coordinated by CNRS/IN2P3 since 2008
- Integration in Geant4 enables the use of Geant4-DNA physics from inside GATE (2014) and TOPAS (2015

How can Geant4-DNA model early DNA damage ?



Brief overview of the Physical stage

- Geant4-DNA physics models are applicable to liquid water –
  - Main component of biological matter
- They can reach the very low energy domain down to electron thermalization
  - Compatible with molecular description of interactions (5 excitation & ionisation levels of the water molecule)
  - Sub-excitation electrons (below ~9 eV) can undergo vibrational excitation, attachment and elastic scattering
- Purely discrete
  - Simulate all elementary interactions on an event-by-event basis (nanometer scale geometries)
  - No condensed history approximation
- Models can be purely analytical and/or use interpolated data tables
  - For eg. computation of integral cross sections
- Can be run in MultiThreading mode from Geant4 10 since December 2013
- They use the same software design as all electromagnetic models available in Geant4 (« standard » and « low energy » EM models and processes)
  - Allows the combination & addition of models and processes
  - Allows combination of discrete/condensed models

The chemical challenge

Geant4

- Simulations with Geant4 are HEP oriented
  - Sequential handling of tracks
  - Simulation based on geometrical space, where interaction length is the main quantity of interest
  - No time synchronization
- No individual molecules
- No Brownian motion

Requirements for RC

- A generic system for handling interactions between tracks
- Molecular species as tracks and targets
- Brownian motion
- Chemical reactions

Chemistry stage

- The dissociative products can recombine to form new chemical species
  - A new stepping algorithm was developed to handle this recombination and more generally manage collisions between tracks
    - Requires the synchronization of tracks during simulation
      - G4VITProcess encapsulates and allows deportation of information related to a track
    - All tracks are transported simultaneously during dynamic or fixed « time steps » – A table of chemical reactions and their reaction rates must be provided
- All parameters are provided through a « Chemistry list » as Geant4 users would do with a « Physics list »
  - G4EmDNAChemistry
  - Note that the chemistry can be started as a standalone application – Input user defined « physics » phase space

Enjoy the examples

Microdosimetry and dnadamage1