Physics and Physics list in Geant4

XII Seminar on Software for Nuclear, Subnuclear and Applied Physics, Porto Conte, Alghero, May 24-29, 2015

Partially based on talks by
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Outline

The philosophy of the physics definition

How to define and activate models

Electromagnetic physics

Hadronic physics

Ongoing models for radiobiology

Philosophy

Provide a general model framework that allows implementation of processes and models

Separate models and cross sections implement processes

MULTIPLE MODELS FOR THE SAME PROCESS

Provide processes containing

Many possible models and cross sections

Default cross sections for each model

Models under continuous development

G4VUserPhysicsList

All physics lists must derive from this class

and then registered with the RunManager

Example

```
class MyPhysicsList: public G4VUserPhysicsList {
public:
MyPhysicsList();
~MyPhysicsList();
void ConstructParticle();
void ConstructProcess();
void SetCuts();
}
```

User must implement the following methods:

ConstructParticle(), ConstructProces(), SetCuts()

ConstructParticle()

Choose the particles you need in your simulation and define all of them here

G4Electron::ElectronDefinition()

G4Gamma::GammaDefinition()

....

Geant4 has classes that create groups of particles

G4BosonConstructor()

G4LeptonConstructor()

....

ConstructProcess()

For each particle defined in ConstructParticle()
assign all the physics processes that you want to consider

```
void MyPhysicsList::ConstructProcess()
{
// provided by G4VUserPhysicsList, assign transportation process to all particles defined in ConstructParticle();
AddTransportation();
ConstructEM()  //Optional
ConstructGeneral() // Optional
………}
```

SetCuts()

Define all production cuts for gamma, electrons and positrons

Recently also for protons

Notice: this is a production cut, not a tracking cut

All particle, once created, are tracked
down to zero kinetic energy

The CUT is used to limit the generation of secondaries
(i.e. delta from ionization, or gamma from bremsstrahlung)

The CUT is expressed in equivalent range

This is converted in energy for each material

Physics definition

Three different way to implement the physics models

Explicitly associating A GIVEN MODEL to a GIVEN PARTICLE in (eventually) a GIVEN ENERGY RANGE

Error prone

At code level

Use of BUILDERS OR CONSTRUCTORS and REFERENCE PHYSICS LISTS

THE CONSTRUCTORS
are process related (Electromagnetic, Hadronic, Elastic, etc.)

THE REFERENCE PHYSICS LISTS are complete physics lists

Can be also called by the macro file

CASE 1: Use of the 'Constructors' and use a modular physics list

- Create a class derived by **G4VModularPhysicsList**
  - **class myList : public G4VModularPhysicsList**
- Implement the mandatory methods **ConstructParticle()** and **ConstructProcess()** and use the appropriate builders (or create your own)

```
void myList::ConstructProcess()
{
  AddTransportation();
  //Em physics
  G4VPhysicsConstructor* emList = new G4EmStandardPhysics();
  emList->ConstructProcess();
  //Inelastic physics for protons
  G4VPhysicsConstructor* pList = new G4QGSPProtonBuilder();
  pList->ConstructProcess();
```

These are 'Constructors'

CASE 2: use of the Reference Physics Lists (already prepared by the collaboration)

- In your main(), just register an instance of the physics list to the **G4RunManager**

```
#include "QGSP_BERT.hh"
int main()
{
  // Run manager
  G4RunManager * runManager = new G4RunManager();

  …
 G4VUserPhysicsList* physics = new QGSP_BERT();
  runManager-> SetUserInitialization(physics);
}
```

Reference physics lists

Provide a complete and realistic physics with ALL models of interest

Provided according to some Use-cases

Few choices are available for EM physics

Several possibilities for hadronic

They are intended as starting point and their builder can be reused

They are made up of builders, so easy to change/replace each given block

Reference physics lists

Electromagnetic interactions for all particles. Different settings are offered

- Default transport parameters (best performance)
- Some optimised choice (_EMV extension)
- Some high precision choice (_EMY extension)

Inelastic interactions

Elastic scattering

Capture

Decay of unstable particles

Specialized treatment of low energy neutrons (< 20 MeV)

Where are the Constructors ?

Where are the builder (or constructors)?

```
constructors Lavora! > pwd
/Users/cirrone/Geant4Dir/geant4-10-00-ref-03/source/physics_lists/constructors
```

```
total 24
-rw-r--r--  1 cirrone  staff   708 Apr 19 00:12 CMakeLists.txt
-rw-r--r--  1 cirrone  staff   870 Apr 19 00:12 GNUmakefile
-rw-r--r--  1 cirrone  staff  1154 Apr 19 00:12 History
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 decay
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 electromagnetic
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 factory
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 gamma_lepto_nuclear
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 hadron_elastic
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 hadron_inelastic
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 ions
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 limiters
drwxr-xr-x  8 cirrone  staff   272 Apr 19 00:12 stopping
```

```
19 00:12 G4EmDNAPhysics.hh
19 00:12 G4EmDNAPhysics_option1.hh
19 00:12 G4EmLivermorePhysics.hh
19 00:12 G4EmLivermorePolarizedPhysics.hh
19 00:12 G4EmLowEPPhysics.hh
19 00:12 G4EmPenelopePhysics.hh
19 00:12 G4EmStandardPhysics.hh
19 00:12 G4EmStandardPhysics_option1.hh
19 00:12 G4EmStandardPhysics_option2.hh
19 00:12 G4EmStandardPhysics_option3.hh
19 00:12 G4EmStandardPhysics_option4.hh
19 00:12 G4OpticalPhysics.hh
19 00:12 G4OpticalPhysicsMessenger.hh
19 00:12 G4OpticalProcessIndex.hh
```

Where are the Physics Lists?


```
lists Lavora! > pwd
/Users/cirrone/Geant4Dir/geant4-10-00-ref-03/source/physics_lists/lists
```

```
-rw-r--r--  1 cirrone  staff  38580 Apr 19 00:12 LBE.icc
-rw-r--r--  1 cirrone  staff   2382 Apr 19 00:12 QBBC.hh
-rw-r--r--  1 cirrone  staff   2509 Apr 19 00:12 QGSP_BERT.hh
-rw-r--r--  1 cirrone  staff   4514 Apr 19 00:12 QGSP_BERT.icc
-rw-r--r--  1 cirrone  staff   2536 Apr 19 00:12 QGSP_BERT_HP.hh
-rw-r--r--  1 cirrone  staff   4332 Apr 19 00:12 QGSP_BERT_HP.icc
-rw-r--r--  1 cirrone  staff   2490 Apr 19 00:12 QGSP_BIC.hh
-rw-r--r--  1 cirrone  staff   4584 Apr 19 00:12 QGSP_BIC.icc
-rw-r--r--  1 cirrone  staff   2544 Apr 19 00:12 QGSP_BIC_HP.hh
-rw-r--r--  1 cirrone  staff   4156 Apr 19 00:12 QGSP_BIC_HP.icc
-rw-r--r--  1 cirrone  staff   2576 Apr 19 00:12 QGSP_FTFP_BERT.hh
-rw-r--r--  1 cirrone  staff   4196 Apr 19 00:12 QGSP_FTFP_BERT.icc
-rw-r--r--  1 cirrone  staff   2186 Apr 19 00:12 QGSP_INCLXX.hh
-rw-r--r--  1 cirrone  staff   2189 Apr 19 00:12 QGSP_INCLXX_HP.hh
-rw-r--r--  1 cirrone  staff   2501 Apr 19 00:12 QGS_BIC.hh
-rw-r--r--  1 cirrone  staff   4353 Apr 19 00:12 QGS_BIC.icc
-rw-r--r--  1 cirrone  staff   2662 Apr 19 00:12 Shielding.hh
-rw-r--r--  1 cirrone  staff   6522 Apr 19 00:12 Shielding.icc
```

```
// EM Physics
this->RegisterPhysics( new G4EmStandardPhysics(ver) );

// Synchroton Radiation & GN Physics
this->RegisterPhysics( new G4EmExtraPhysics(ver) );

// Decays
this->RegisterPhysics( new G4DecayPhysics(ver) );

 // Hadron Elastic scattering
this->RegisterPhysics( new G4HadronElasticPhysics(ver) );

 // Hadron Physics
this->RegisterPhysics(  new G4HadronPhysicsQGSP_BIC(ver));

// Stopping Physics
this->RegisterPhysics( new G4StoppingPhysics(ver) );

// Ion Physics
this->RegisterPhysics( new G4IonPhysics(ver));

// Neutron tracking cut
this->RegisterPhysics( new G4NeutronTrackingCut(ver));
```

Electromagnetic Physics

EM concepts I

The same physics processes (e.g. Compton scattering) can be described by different models, that can be alternative or complementary in a given energy range

For instance: Compton scattering can be described by

- G4KleinNishinaCompton
- G4LivermoreComptonModel (specialized low-energy, based on the Livermore database)
- G4PenelopeComptonModel (specialized low-energy, based on the Penelope analytical model)
- G4LivermorePolarizedComptonModel (specialized low-energy, Livermore database with polarization)
- G4PolarizedComptonModel (Klein-Nishina with polarization)

Different models can be combined, so that the appropriate one is used in each given energy range (performance optimization)

EM concepts II

A physical interaction or process is described by a process class

Naming scheme : « G4ProcessName »

Eg. : « **G4Compton** » for photon Compton scattering

A physical process can be simulated according to several models, each model being described by a model class

Naming scheme is: « G4ModelNameProcessNameModel »

Eg. : « **G4LivermoreComptonModel** » for the Livermore Compton model

Models can be alternative and/or complementary on certain energy ranges

Refer to the Geant4 manual for the full list of available models

EM physics models

Models and processes for the description of the EM interactions in Geant4 have been grouped in several packages

Package	Description
Standard	γ-rays, $e^{\pm}$ up to 100 TeV, Hadrons, ions up to 100 TeV
Muons	Muons up to 1 PeV
X-rays	X-rays and optical photon production
Optical	Optical photons interactions
High-Energy	Processes at high energy (> 10 GeV). Physics for exotic particles
Low-Energy	Specialized processes for low-energy (down to 250 eV), including atomic effects
Polarization	Simulation of polarized beams

EM processes for gamma and e+/-

Particle	Process	G4Process
Photons	Gamma Conversion in $e^{\pm}$	`G4GammaConversion`
	Compton scattering	`G4ComptonScattering`
	Photoelectric effect	`G4PhotoElectricEffect`
	Rayleigh scattering	`G4RayleighScattering`
$e^{\pm}$	Ionisation	`G4eIonisation`
	Bremsstrahlung	`G4eBremsstrahlung`
	Multiple scattering	`G4eMultipleScattering`
e^{+}	Annihilation	`G4eplusAnnihilation`

When/why to use Low Energy models

Use Low-Energy models (Livermore or Penelope), as an alternative to Standard models, when you:

- need precise treatment of EM showers and interactions at low-energy (keV scale)
- are interested in atomic effects, as fluorescence x-rays, Doppler broadening, etc.
- can afford a more CPU-intensive simulation
- want to cross-check another simulation (e.g. with a different model)

Do not use when you are interested in EM physics at the MeV region

- same results as Standard EM models, performance penalty

Example: physics list for gamma


```
G4ProcessManager* pmanager
if ( particleName == "gamma"   )
{
 pmanager->AddDiscreteProcess(new G4PhotoElectricEffect);
 pmanager->AddDiscreteProcess(new G4ComptonScattering);
 pmanager->AddDiscreteProcess(new G4GammaConversion);
 pmanager->AddDiscreteProcess(new G4RayleighScattering);
}
```

Single and multiple scattering

Model	Particle type	Energy limit	Specifics and applicability
Urban (Urban 2006)	Any	-	Default model for electrons and positrons below 100 MeV, (Lewis 1950) approach, tuned to data, used for LHC production.
Screened Nuclear Recoil (Mendenhall and Weller 2005)	p, ions	< 100 MeV/A	Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space app.
Goudsmit-Saunderson (Kadri 2009)	e^+, e^-	< 1 GeV	Theory based cross sections (Goudsmit and Saunderson 1950). EPSEPA code developed by Penelope group, final state using EGSnrc method (Kawrakov et al. 1998), precise electron transport
Coulomb scattering (2008)	any	-	Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons
WentzelVI (2009)	any	-	MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons.
Ion Coulomb scattering (2010) Electron Coulomb scattering (2012)	Ions e^+, e^-	-	Model based on Wentzel formula + relativistic effects + screening effects for projectile & target. From the work of P. G. Rancoita, C. Consolandi and V. Ivantchenko.

Single and multiple scattering

Multiple scattering (class name `G4UrbanMscModel`)

Multiple scattering (class name `G4WentzelVIModel`)

Multiple scattering (class name `G4LowEWentzelVIModel`)

Alternative process for simulation of single Coulomb scattering of all charged particles (class name `G4CoulombScattering`)

Alternative process for simulation of single Coulomb scattering of ions (class name `G4ScreenedNuclearRecoil`)

Ready-to-use Physics Constructors

G4EmStandardPhysics – default
G4EmStandardPhysics_option1 – HEP fast but not precise
G4EmStandardPhysics_option2 – Experimental
G4EmStandardPhysics_option3 – medical, space
G4EmLivermorePhysics
G4EmLivermorePolarizedPhysics
G4EmPenelopePhysics
G4EmDNAPhysics

Combined Physics
Standard > 1 GeV
LowEnergy < 1 GeV

- **`$G4INSTALL/source/physics_list/builders`**
- Advantage of using of these classes – they are tested on regular basis and are used for regular validation

How to extract physics

Possible to retrieve physics quantities via the G4EmCalculator class file

Example for retrieving total cross section of a process with name procName, for particle partName and for the material matName

```
G4EmCalculator emCalculator;
G4Material* material =
  G4NistManager::Instance()->FindOrBuildMaterial("matName);
G4double massSigma = emCalculator.ComputeCrossSectionPerVolume
   (energy,particle,procName,material);
G4cout << G4BestUnit(massSigma, "Surface/Volume") << G4endl;
```

See $G4INSTALL/examples/extended/electromagnetic/TestEm14

Hadronic physics coins

Hadronic Physics

Data-driven models

Parametrisation models

Theory driven models

Hadronic physics challenge

Three energy regimes

< 100 MeV

resonance and cascade region (100 MeV - 10 GeV)

> 20 GeV (QCD strings)

Within each regime there are several models

Many of these are phenomenological

Reference physics lists for Hadronic interaction

Are part of the Geant4 code

Three family of lists

- QGS, or list based on a model that use the Quark Gluon String model for high energy hadronic interactions of protons, neutrons, pions and kaons
- FTF, based on the FTF (FRITIOF like string model) for protons, neutrons, pions and kaons
- Other specialized physics lists

Cross sections

Default Cross sections but also specific databases:

- Low energy neutrons
  - G4NDL available as external data files
  - Available with or without thermal cross section
- Neutron and proton reaction cross section
  - 20 MeV < E < 20 GeV
- Ion-nucleus reaction cross sections
  - E/A < 1 GeV
- Isotope production data

G4NDL (G4 Neutron Data Library)

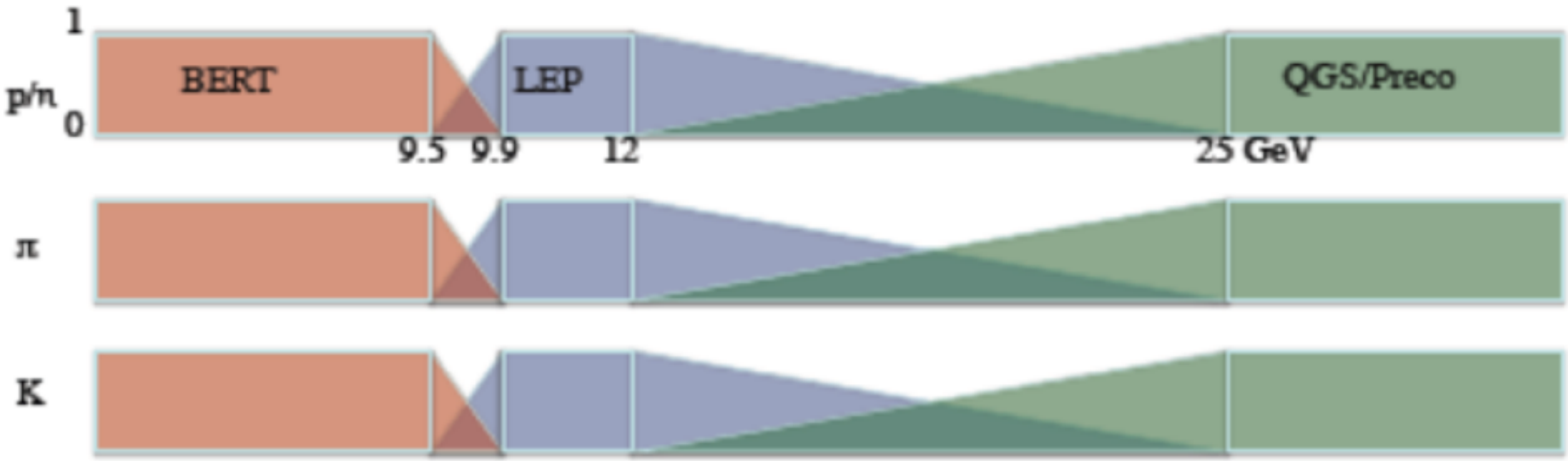
Neutron data files for High precision models

These data include both cross sections and final states

These data derived by the following evaluated data libraries

- Brond-2.1
- CENDL2.2
- EFF-3
- ENDF/B
- FENDL/E
- JEF2.2
- JENDL-FF
- MENDL

Hadronic models match



Recommended reference physics lists

A dedicated web page

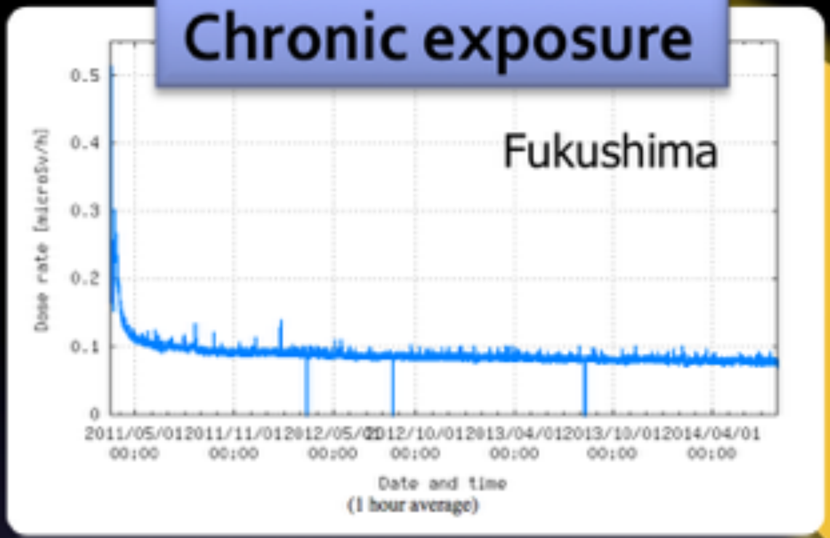
Application fields are identified

- High energy physics
- LHC neutron fluxes
- Shielding
- Medical
- ....

Geant4-DNA coins

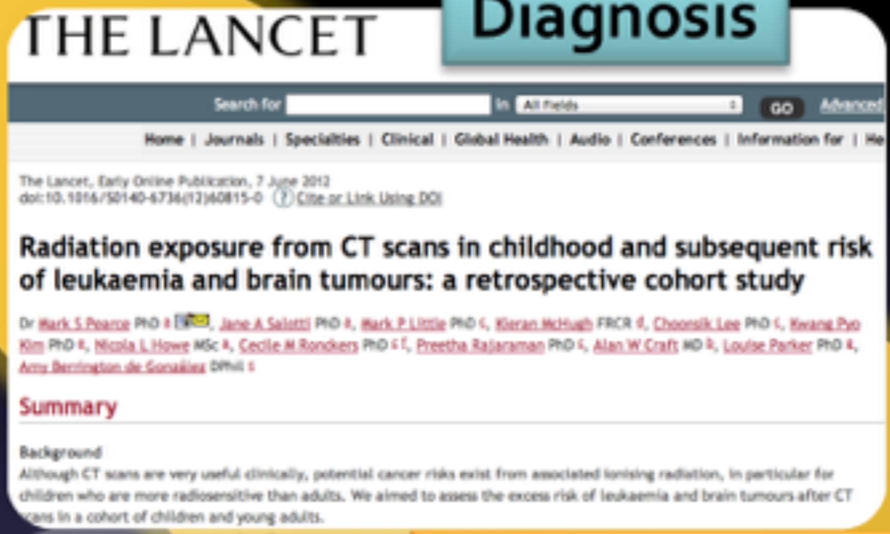
Modelling biological effects of ionising radiation remains a major scientific challenge

Chronic exposure



http://rcwww.kek.jp/norm/index-e.html

Diagnosis



THE LANCET

The Lancet, Early Online Publication, 7 June 2012
doi:10.1016/S0140-6736(12)60815-0 Cite or Link Using DOI

Radiation exposure from CT scans in childhood and subsequent risk of leukaemia and brain tumours: a retrospective cohort study

Dr Mark S Pearce PhD, Jane A Salotti PhD, Mark P Little PhD, Kieran McHugh FRCR, Choonsik Lee PhD, Kwang Pyo Kim PhD, Nicola L Howe MSc, Cecile M Ronckers PhD, Preetha Rajaraman PhD, Alan W Craft MD, Louise Parker PhD, Amy Berrington de González DPhil

Summary

Background

Although CT scans are very useful clinically, potential cancer risks exist from associated ionising radiation, in particular for children who are more radiosensitive than adults. We aimed to assess the excess risk of leukaemia and brain tumours after CT scans in a cohort of children and young adults.

Space missions

Space exploration

Proton & hadrontherapy

« A major challenge lies in providing a sound mechanistic understanding of low-dose radiation carcinogenesis »

L. Mullenders *et al.*

Assessing cancer risks of low-dose radiation

Nature Reviews Cancer (2009)

G4-DNA

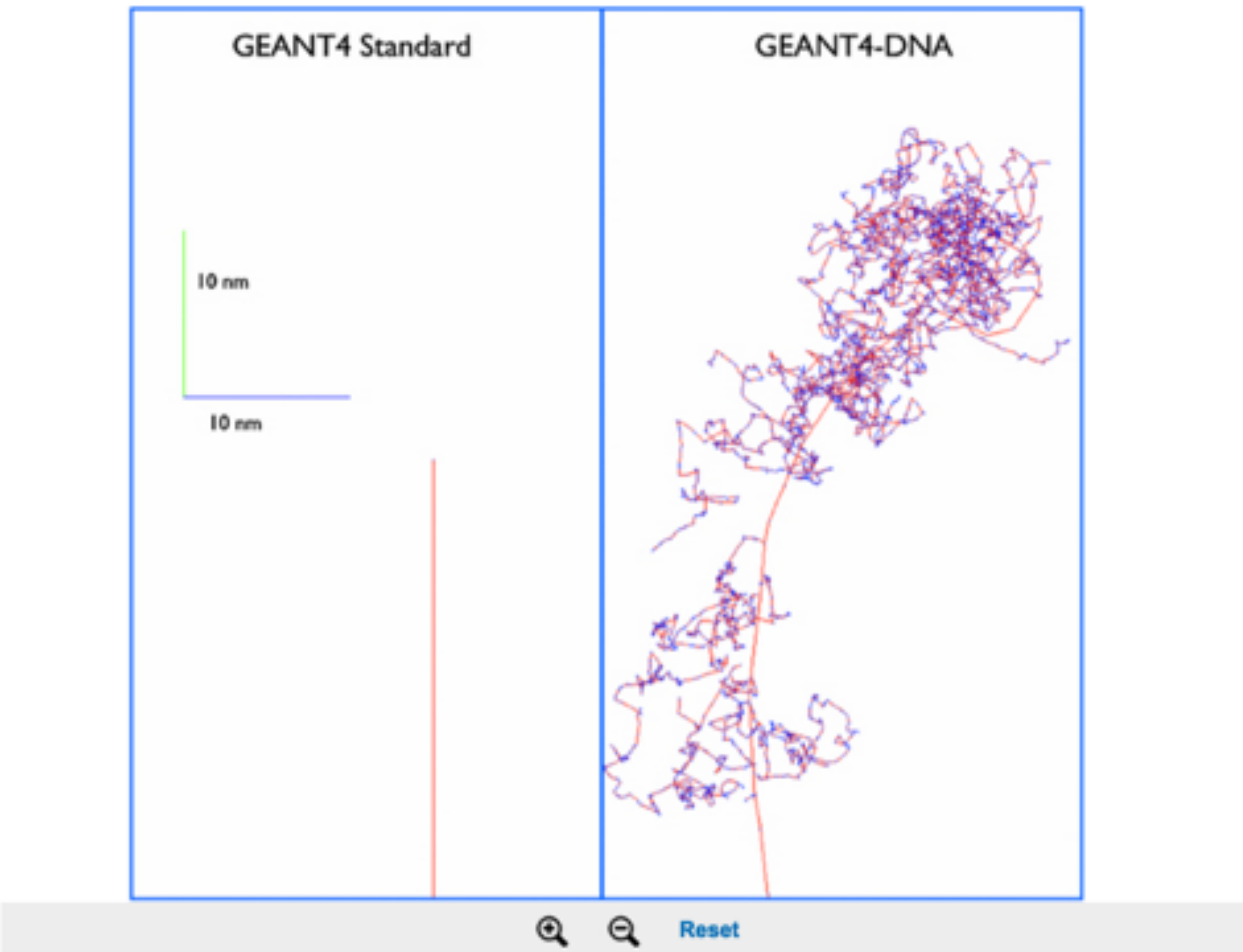


Figure 4. Two 1 keV electrons incident on slab of liquid water using: (*left*) GEANT4 standard electromagnetic processes, (*right*) GEANT4-DNA low energy processes. The standard processes kill the electron after one interaction and deposit its energy locally. The GEANT4-DNA processes explicitly simulate every interaction, elastic scattering, ionizations and excitations down to 5 eV in this simulation, where the electron energy is deposited locally.

Simulation at the DNA level

`examples/extended/medical/dna/dnaphysics`

Monte Carlo role in radiobiological modelling of radiotherapy outcomes

FREE ARTICLE REVIEW ARTICLE

Issam El Naqa, Piotr Pater and Jan Seuntjens

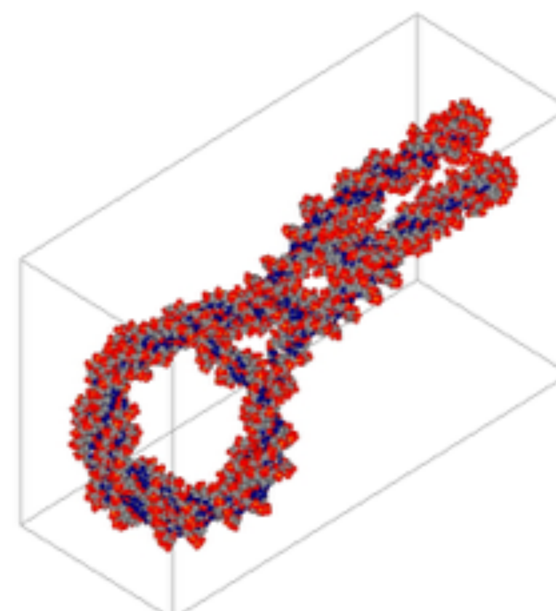
Show affiliations

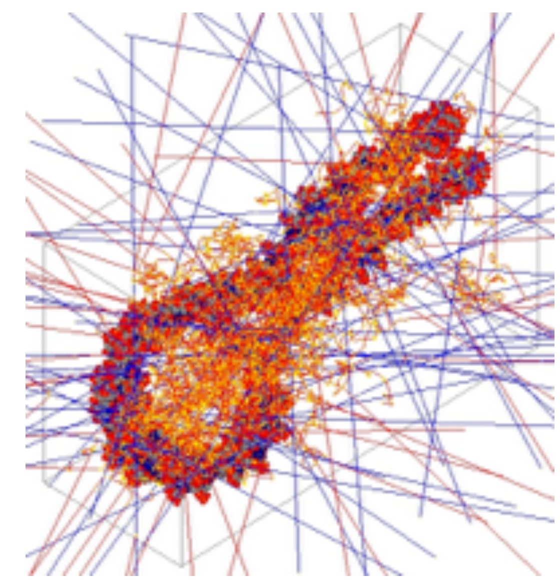
Issam El Naqa *et al* 2012 *Phys. Med. Biol.* **57** R75

doi:10.1088/0031-9155/57/11/R75

Using Protein Data Bank files

`examples/extended/medical/dna/pdb4dna`





G4-DNA

Monte Carlo approach for radiobiology at micro and nano scale

Many Monte Carlo codes are already available today in radiobiology for the simulation of track structures at the molecular scale in biological medium

E.g. PARTRAC, TRIOL, PHITS, KURBUC, NOREC...

Include physics & physico-chemistry processes, detailed geometrical descriptions of biological targets down to the DNA size, DNA and chromosome damage simulation and even repair mechanisms (PARTRAC)...

Usually designed for very specific applications

Not always easily accessible

- Is it possible to access the source code ?
- Are they adapted to recent OSs ?
- Are they extendable by the user ?

« To expand accessibility and avoid 'reinventing the wheel', track structure codes should be made available to all users via the internet from a central data bank»

H. Nikjoo, IJRB 73, 355 (1998)

G4-DNA

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

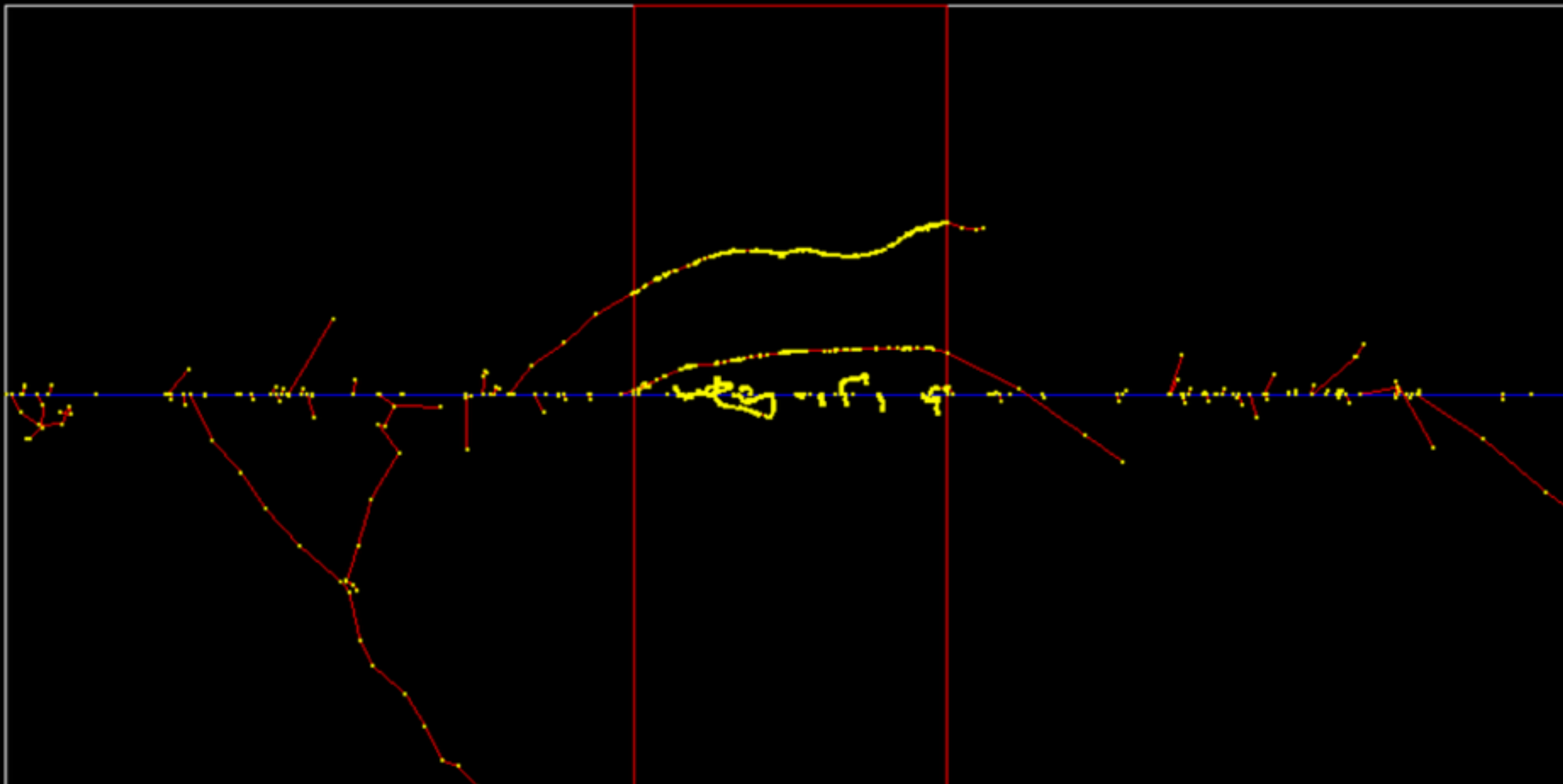
- Condensed-history approach
  - No step-by-step transport on small distances, a key requirement for micro/nano-dosimetry
- Low-energy limit applicability of EM physics models is limited
  - Livermore Low Energy EM models can technically go down to 10 eV but accuracy limited
  - 100 eV for Penelope 2008 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...

G4-DNA

- 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

Thanks to S Incerti

Geant4 EM standard physics | Geant4-DNA | Geant4 EM standard physics



/gps/particle ion
/gps/ion 6 12 6
/gps/energy 240 MeV

Courtesy of V. Stepan (CENBG)

See NIMB 273 (2012) 95-97 (link)
Prog. Nucl. Sci. Tec. 2 (2011) 898-903 (link)

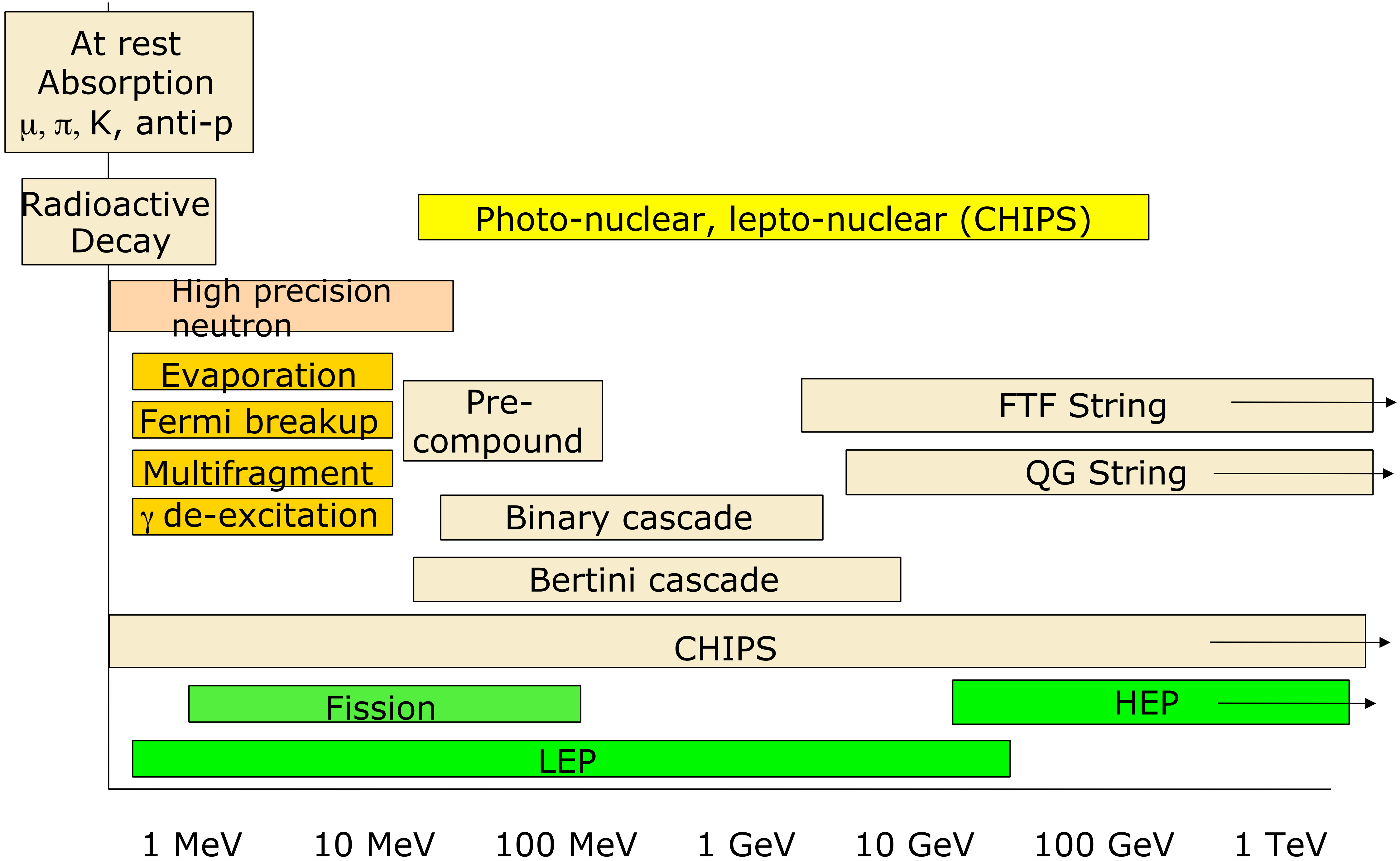
G4-DNA


```
~ Lavora! > cd Geant4Dir/geant4-10-01-ref-00/source/processes/electromagnetic/
electromagnetic Lavora! > ll
total 24
-rw-r--r--   1 cirrone  staff   676 Dec  5 16:27 CMakeLists.txt
-rw-r--r--   1 cirrone  staff   857 Dec  5 16:27 GNUmakefile
-rw-r--r--   1 cirrone  staff  2738 Dec  5 16:27 History
drwxr-xr-x   8 cirrone  staff   272 Dec  5 16:27 adjoint
drwxr-xr-x  11 cirrone  staff   374 Dec  5 16:27 dna
drwxr-xr-x   8 cirrone  staff   272 Dec  5 16:27 highenergy
drwxr-xr-x   9 cirrone  staff   306 Dec  5 16:27 lowenergy
drwxr-xr-x   8 cirrone  staff   272 Dec  5 16:27 muons
drwxr-xr-x   8 cirrone  staff   272 Dec  5 16:27 pii
drwxr-xr-x   8 cirrone  staff   272 Dec  5 16:27 polarisation
drwxr-xr-x   9 cirrone  staff   306 Dec  5 16:27 standard
drwxr-xr-x   9 cirrone  staff   306 Dec  5 16:27 utils
drwxr-xr-x   9 cirrone  staff   306 Dec  5 16:27 xrays
```

```
-rw-r--r--  1 cirrone  staff    586 Dec  5 16:27 CMakeLists.txt
-rw-r--r--  1 cirrone  staff    561 Dec  5 16:27 GNUmakefile
-rw-r--r--  1 cirrone  staff  27724 Dec  5 16:27 History
drwxr-xr-x  8 cirrone  staff    272 Dec  5 16:27 management
drwxr-xr-x  7 cirrone  staff    238 Dec  5 16:27 models
drwxr-xr-x  7 cirrone  staff    238 Dec  5 16:27 molecules
drwxr-xr-x  7 cirrone  staff    238 Dec  5 16:27 processes
drwxr-xr-x  6 cirrone  staff    204 Dec  5 16:27 test
drwxr-xr-x  7 cirrone  staff    238 Dec  5 16:27 utils
dna Lavora! >
```

Hadronic process/Model Inventory

http://geant4.cern.ch/support/proc_mod_catalog/models



Where to find information?

Process/model catalog

Home/User Support --> Geant4 web site

Where to find information?

User Support

1. Getting started
2. Training courses and materials
3. Source code
   a. Download page
   b. LXR code browser -or- draft doxygen documentation
4. Frequently Asked Questions (FAQ)
5. Bug reports and fixes
6. User requirements tracker
7. User Forum
8. Documentation
   a. Introduction to Geant4
   b. Installation Guide
   c. Application Developers Guide
   d. Toolkit Developers Guide
   e. Physics Reference Manual
   f. Software Reference Manual
9. Physics lists
   a. Electromagnetic
   b. Hadronic

Thank you