Report on session 3A

« New EM developments »

7 talks

Firsov and Remizovich effects for low energy low angle proton scattering simulation *MANTERO, Alfonso et al.*

New evaluated PIXE model from ANSTO *GUATELLI, Susanna*

Aula Magna, Ferrara 14:15 - 14:30

New developments of MicroElec processes for low-energy electron transport in Al, Ag and Si *INGUIMBERT, Christophe*

Flagged uniform particle split for Geant4-DNA *RAMOS-MENDEZ, Jose*

Aula Magna, Ferrara 14:45 - 15:00

MPEXS-DNA, a GPU implementation of Geant4-DNA *OKADA, Shogo*

Aula Magna, Ferrara 15:00 - 15:15

A Geant4 application for flexible and extendable DNA geometries incorporating physical and chemical genome damage *LAMPE, Nathanael*

Evaluation of radio-induced DNA damages simulating the physical, physico-chemical and chemical stages with Geant4-DNA *MEYLAN, Sylvain*

1) A model for grazing angles soft proton scattering

A. Mantero, P. Dondero et al.

- @ 250 keV, Remizovich and SS consistent with exp data except below < 1 deg.
- SS is the closest to the observation for LowEn, BUT
  - Energy loss is 10 times lower
- MSC good for high energy, both for scattering and energy loss
- @ "large" incident angles all the models are consistent
  - the angular distribution does not depend on p energy
- Firsov (φ = 0 Remizovich integration) overestimates 10 times exp data
- no differences are found between the EM opt3 and opt4 list multiple scattering settings.

More to do:
- **Full Remizovich implementation**
- Computing efficiency
- Geant4 integration

More work needed:
- Ad-Hoc measurements
  - Structures
  - Funding

2) The ANSTO Evaluated PIXE Model

CMRP: S. Guatelli and S. Bakr, ANSTO: D. Cohen and R. Siegele, Swhard: A. Mantero and P. Dondero, CENBG: S. Incerti

- New project

- Import in Geant4 the ANSTO Evaluated PIXE model
  - By J. Crawford, D. Cohen, R. Siegele, G. Doherty, A. Atanacio
  - Up to 5 MeV proton energy
  - Data available also for deuterium and helium as incident particles
  - Targets with Z between 6 and 92
  - Data provided within a self-consistent database, validated against experimental measurements

- Compare the alternative Geant4 PIXE models against experimental measurements of ANSTO micro-PIXE facility

Australian Government | ansto | CENBG | SWHARD Cuttin'Edge Technology

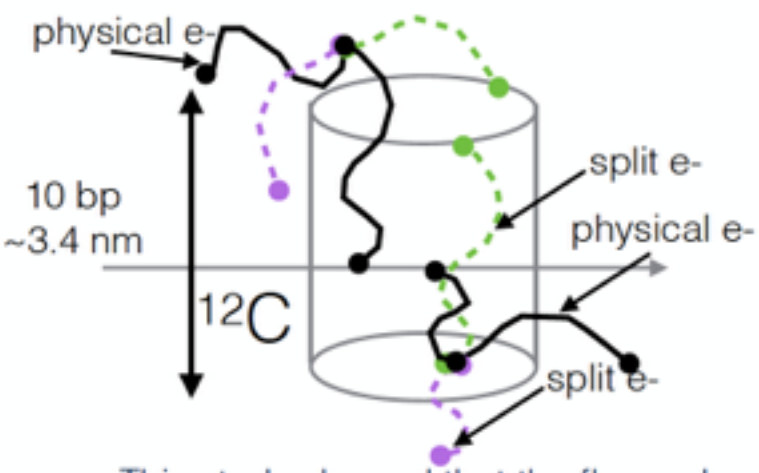
3) New developments for MicroElec (Al, Ag, Si)

C. Inguimbert, M. Raine

	OSMOSEE	Geant4	Status	On going work
Date	2011	June 2012	**September 2016**	
Material	Al	Si	**Si, Al implemented** Cross section also calculated for Ag	Ag must be tabulated in MicroElec format
Energy range	10 eV – 5 keV	16,7 eV–100 MeV		
Inelastic model	**Specific for each interaction in Al. ~4 eV**	GLOBAL Dielectric function Formalism **16,7 eV**	**Inelastic cross section Down to ~1 eV in Si, Al**	
Elastic model	Mott-ELSEPA **10 eV but all Z** [4]	ICRU [6] database **5eV for Si only**	**Elastic cross section Down to 5 eV in Si and Al**	Ag must be tabulated in MicroElec format
Geometry	No complex 3D	G4 3D	**Available for all Z (NIST)**	
Material interfaces	Vacuum/Al + surface plasmon	**none**		**Vacuum/material interface not yet included**
Phonons	Simplistic approach	**none**	Some comparisons with experimental electron secondary emission yield have been performed	Phonons not yet implemented
Observables	**S**econdary **E**lectron **E**mission **-SEE** Yield -Energetic spectrum -Angular distribution	User defined Track structure of heavy ions		

4) Flagged uniform particle split for Geant4-DNA

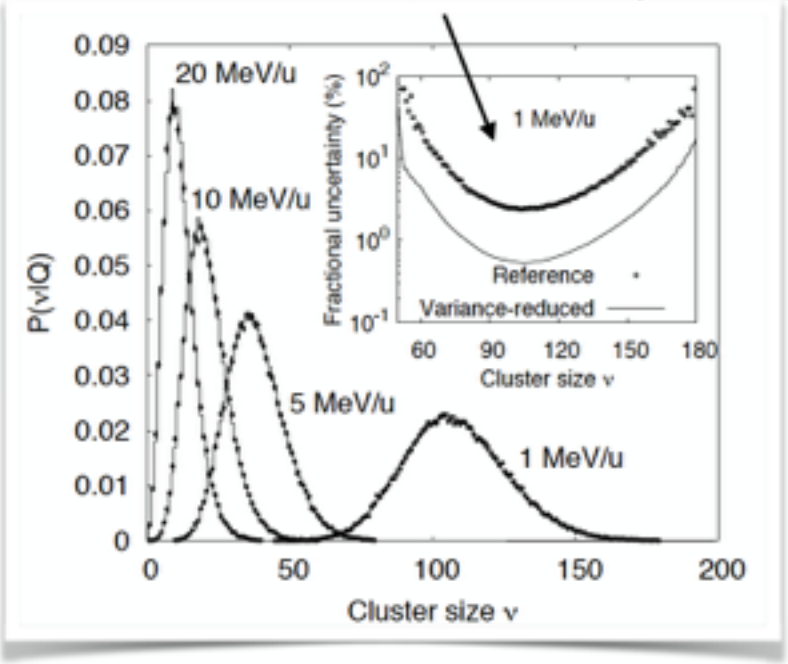
J. Ramos-Mendez, B. Faddegon



- Uniform splitting is applied to e-_G4DNAIonisation via G4WrapperProcess
- A unique flag (integer number) is assigned to each new split particle.
- This flag must be **inherited** to all subsequent secondaries.
- Use this flag to classify all the tracks independently

- This study showed that the flagged uniform particle split allows to achieve significant improvement of the computational efficiency of Geant4-DNA simulations without compromising the accuracy.
- For protons, the relative efficiency ranged from **50 to 350** (less complex scoring, high to low LET). For carbon ions, the relative efficiency ranged from about **45 to 55** (simple scoring, high to low LET). In both scenarios, the relative differences between variance-reduced and reference simulations were within the 2% within the statistical uncertainty.

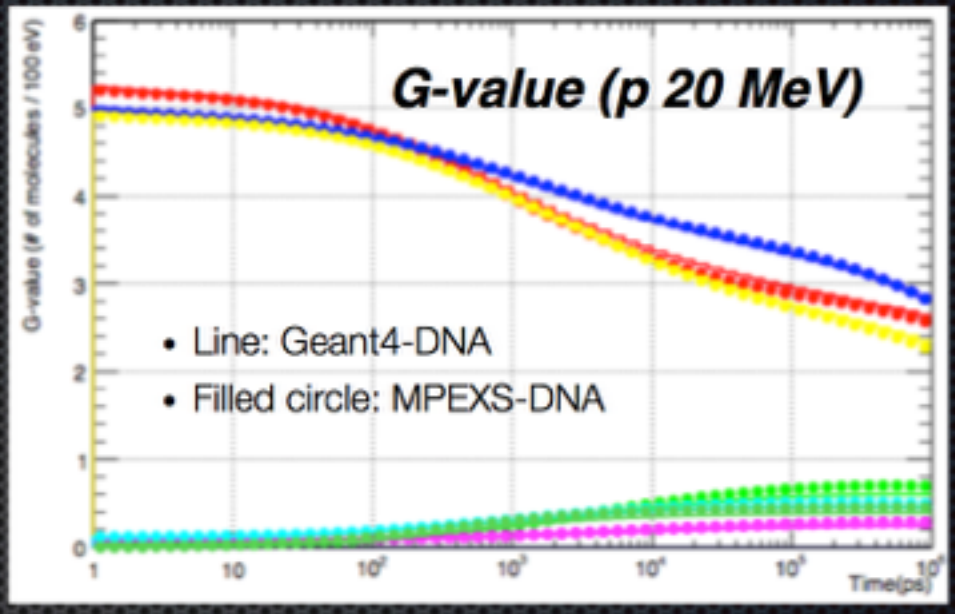
Same execution time (N_s=32)



5) MPEXS-DNA, a GPU implementation of Geant4-DNA Summary

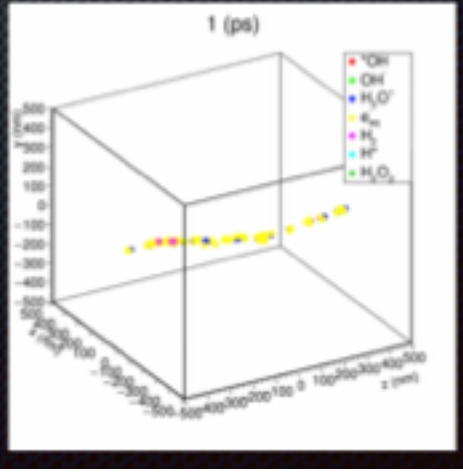
S. Okada et al.

- DNA Physics and Chemical simulation can be run on GPU
  - Geant4-DNA processes are implemented in CUDA
  - MPEXS-DNA have the same accuracy as Geant4-DNA



- **Achieve up to 200 times speedup agains single-core CPU**
  - ~ 2.5 days (CPU) -> ***~ 20 min. (GPU)*** (ex. p 20 MeV, 10k events)

	e- 10 keV	e- 750 keV	p 20 MeV
Water phantom size	1 x 1 x 1 um	5 x 5 x 5 um	1 x 1 x 1 um
Average # of molecules generated at 1 ps	419	126	347
Process time (Geant4-DNA 10.02 p01)	30.6 sec / event	5.01 sec / event	22.1 sec / event
Process time (MPEXS-DNA)	0.197 sec / event	0.0336 sec / event	0.115 sec / event
Speedup factor	***155x***	***149x***	***192x***

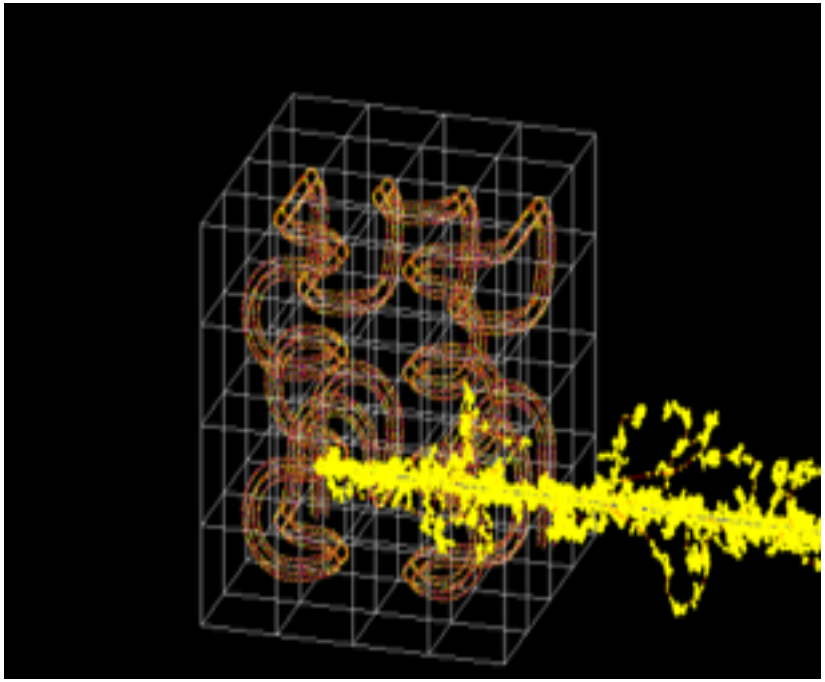


6) The MolecularDNA Application

N. Lampe

- A monolithic application simulating direct and indirect DNA damage
- Flexible specification of DNA geometries
  - Ships with bacterial DNA
  - Extendable to chromatin, plasmids, test DNA geometries, all without touching C++
- Coming early 2017

1 MeV protons travelling through a simple continuous DNA model



7) Evaluation of radio-induced DNA damages simulating the physical, physico-chemical and chemical stages with Geant4-DNA

S. Meylan

- **DnaFabric**
  - ✓ Generate/Edit/Save complex DNA geometries
  - ✓ Visualize
  - ✓ Export to Geant4-DNA (".fab2g4dna" file)

- **Simulate the physical, physico-chemical and chemical stages with such geometrical models.**

- **Results are consistent** with experimental data

- **Criteria associated with the creation of DNA damages are not "set in stone":**
  - ➢ Direct SSB threshold or linear acceptation probability
  - ➢ Duration of the chemical stage (by default 2.5 ns).

What will be delivered:

- ✓ A user-application to show how to introduce a DNA geometrical model in a chemical simulation.
- ✓ To do so, some of the Geant4 modifications should be integrated.