Development of chemistry and biodose actors in GATE 10

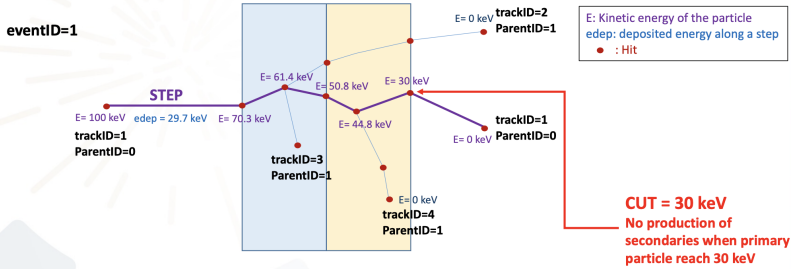
Alexis Pereda[1], Hermann Fuchs[4], Dietmar Georg[4], Jean Michel Létang[2], Étienne Testa[3], Michael Beuve[3], Lydia Maigne[1], Geant4-DNA collaboration
[1]LPCA, [2]CREATIS, [3]IP2I, [4]Medical University of Vienna/MedAustron

<alexis.pereda@clermont.in2p3.fr>

Laboratoire de Physique Clermont Auvergne, UCA, CNRS, France

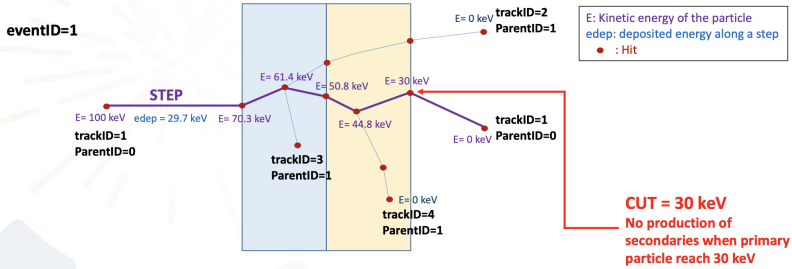
GATE Scientific Meeting 2025

GATE



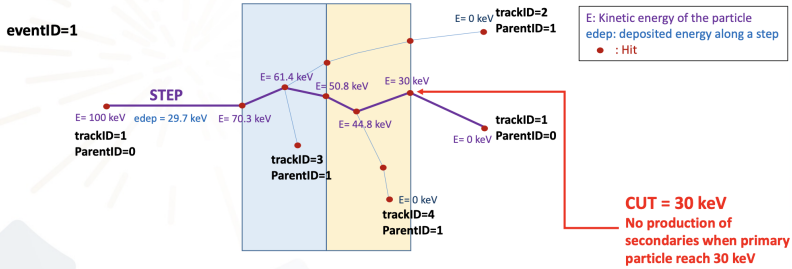
	Geant4 actions					
	`BeginOfRun`	`BeginOfEvent`	`Stepping`	`EndOfEvent`	`EndOfRun`	`NewStage`
compute dose	✓		✓		✓	
compute fluence	✓	✓	✓		✓	
compute biodose	✓	✓	✓	✓	✓	
apply chemistry				✓	✓	✓

GATE



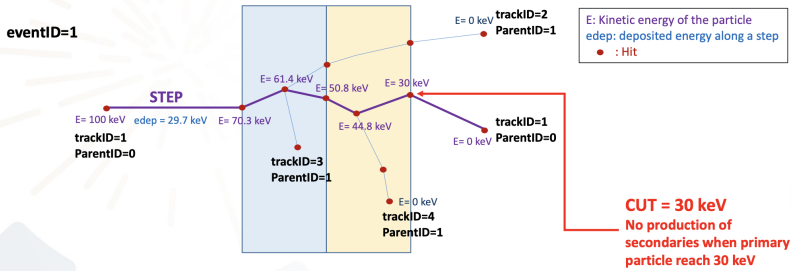
	Geant4 actions					
	BeginOfRun	BeginOfEvent	Stepping	EndOfEvent	EndOfRun	NewStage
compute dose	✓		✓		✓	
compute fluence	✓	✓	✓		✓	
compute biodose	✓	✓	✓	✓	✓	
apply chemistry				✓	✓	✓

GATE



	Geant4 actions					
	`BeginOfRun`	`BeginOfEvent`	`Stepping`	`EndOfEvent`	`EndOfRun`	`NewStage`
compute dose	✓		✓		✓	
compute fluence	✓	✓	✓		✓	
compute biodose	✓	✓	✓	✓	✓	
apply chemistry				✓	✓	✓

GATE



	Geant4 actions					
GATE actors ↓	`BeginOfRun`	`BeginOfEvent`	`Stepping`	`EndOfEvent`	`EndOfRun`	`NewStage`
DoseActor	✓		✓		✓	
FluenceActor	✓	✓	✓		✓	
BioDoseActor	✓	✓	✓	✓	✓	
ChemistryActor				✓	✓	✓

Biological dose

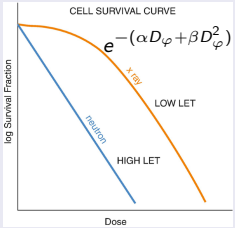
Objective of the biological dose

effects of the physical dose on biological tissues

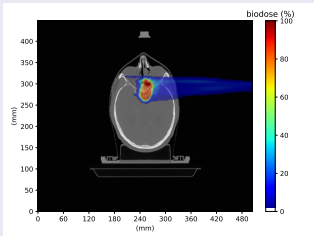
nano/micro scale

- mMKM
  (Kase et al., 2006)
- NanOx
  (Cunha et al., 2017)

cellular scale



macro scale



Biophysical model databases

Cell line Human Salivary Glands (HSG): `HSG_mMKM.db` or `HSG_NanOx.db`
$\Longrightarrow$ easy to provide new cell lines or biophysical models

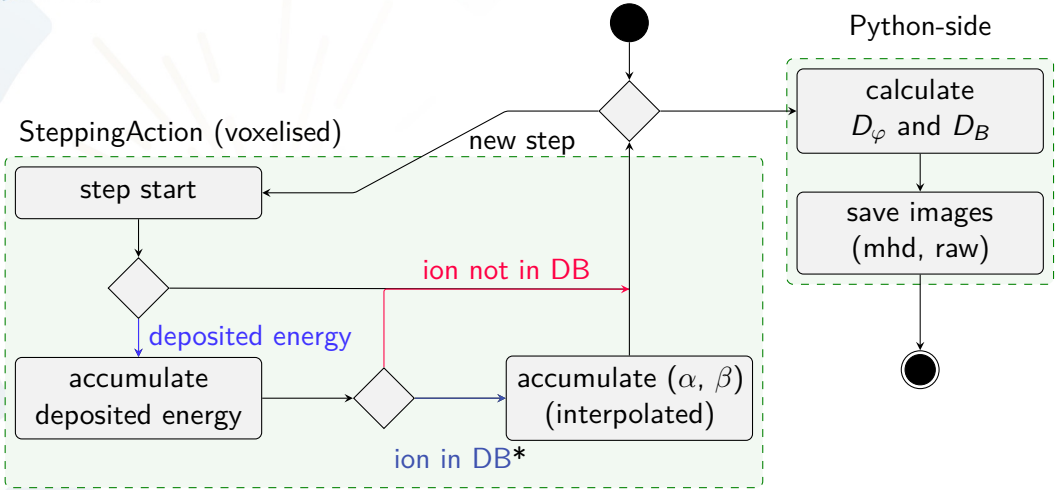
Example:

α, β: from Geant4-DNA/LPCHEM simulations

```
// Ion type

H
...
He
...
C
...
O
...
Li
...
```

```
// energy   alpha    beta
// (MeV)    (Gy-1)   (Gy-2)
H
0.1         3.528    0.059
0.125       3.584    0.022
0.15        3.642    0.098
...
1           0.932    0.059
...
10          0.376    0.063
...
300         0.339    0.109
```

BioDoseActor process diagram

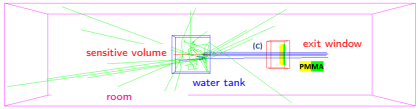


* provided databases (DB) contain values for {H, He, C, O, Li}

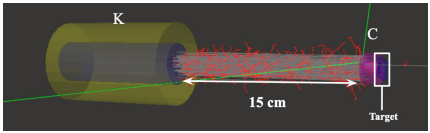
User interface

```
biodose = sim.add_actor("BioDoseActor", "biodose")

biodose.attached_to          = volume
biodose.output_filename      = "biodose.mhd"
biodose.translation          = [0, 0, 0]
biodose.spacing              = [1 * mm, 60 * mm, 60 * mm]
biodose.size                 = [400, 1, 1]

biodose.cell_line            = "HSG"
biodose.biophysical_model    = "NanOx"
biodose.alpha_ref            = 0.313
biodose.beta_ref             = 0.0615
biodose.uncertainty.active   = True
```

Clinical and pre-clinical simulations



- Pencil Beam Scanning:
  - H: 95.9 – 113 MeV
  - C: 120 – 402 MeV/u
- PhysicsList:
  - H: `QGSP_BIC_EMZ`
  - C: `Shielding_EMZ`



- Pulsed beam:
  - He^{2+}: 67 MeV
- PhysicsList: `G4EmDNAPhysics_option2`

Results – dose profiles

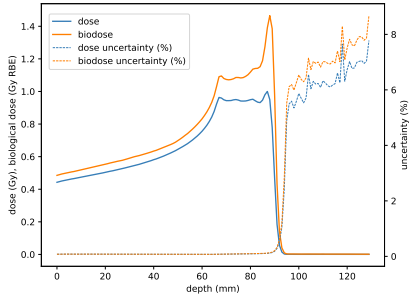


Figure: H-ion in water with 1×10^7 primaries, production cut 100 m, step limiter 10 µm (HSG, NanOx)

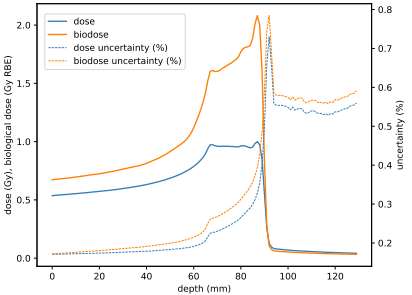
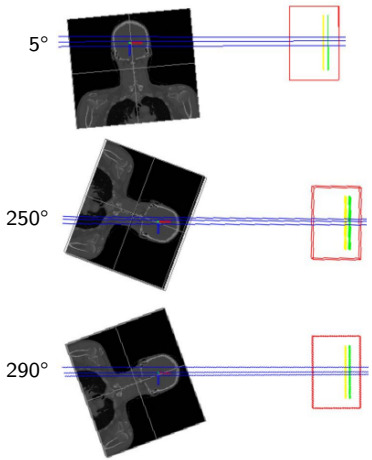


Figure: C-ion in water with 1×10^6 primaries, production cut 100 m, step limiter 10 µm (HSG, mMKM)

MedAustron

C-ion clinical PBS beams in patient

- Human Salivary Glands
- Pencil Beam Scanning
- CT: $50 \times 50 \times 44$ cm^3
- Voxel size: $0.97 \times 0.97 \times 2$ mm^3
- PhysicsList: `Shielding_EMZ`
- 3 beams
- sinonasal chordoma



Results – C-ion, biological dose (NanOx)

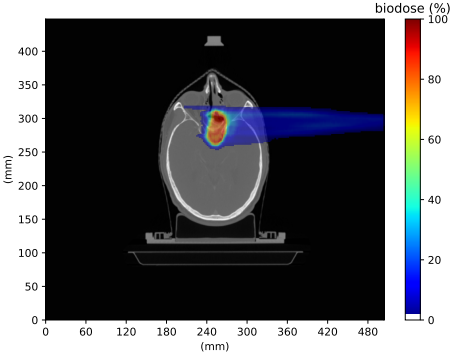


Figure: biological dose with C-ion in patient, 1×10^6 primaries per beam, production cut 100 m, step limiter 10 µm (HSG, NanOx)

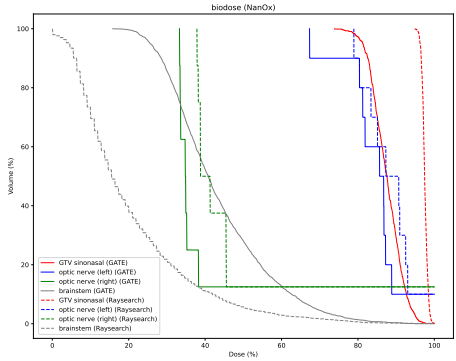


Figure: Cumulative biological DVH comparison GATE/NanOx (solid lines) and Raysearch (dashed lines)

Results – Arronax Helium SOBP (NanOx)

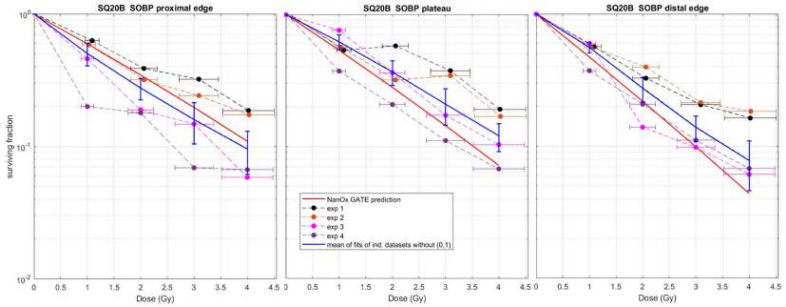
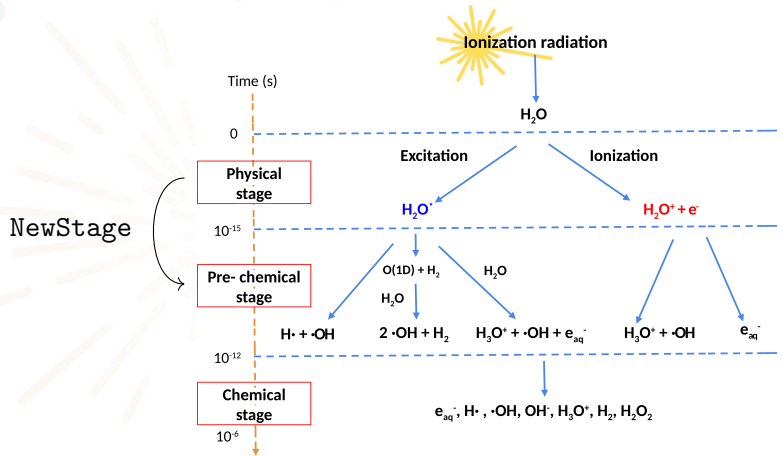


Figure: Irradiation of SQ20B (Human Squamous Cell Carcinoma) cells in a helium SOBP: comparison of measured surviving fractions with NanOx predictions for three irradiation settings (Berger et al., in preparation).

Slide content by Mario Alcocer (Berger et al.) [preliminary results]

Geant4-DNA chemistry



Main figure from Da Eun Kwon (Ph.D. student)

Chemistry in GATE

Main purpose

Being able to use Geant4-DNA chemistry directly in GATE
(e.g. to study water radiolysis for FLASH therapy)

This requires:

- handling physics/chemistry lists
- triggering the chemical stage
- new user code to record chemical reactions
- (wip) being able to configure the simulation (pH, scavengers, ...)
- (wip) output handling

Chemistry lists

```
sim = gate.Simulation()

# G4EmDNAPhysics, G4EmDNAPhysics_option1..8
sim.physics_manager.physics_list_name = "G4EmDNAPhysics_option2"

# G4EmDNAChemistry, G4EmDNAChemistry_option1..4
sim.physics_manager.chemistry_list_name = "G4EmDNAChemistry_option3"
```

Chemistry actor – interface

```
chemistry = sim.add_actor("ChemistryActor", "chemistry")
chemistry.attached_to     = volume
chemistry.timestep_model  = "IRT"  # "IRT", "IRT_syn", "SBS"
chemistry.end_time        = 1 * ns
chemistry.time_bins_count = 50
chemistry.pH              = 7
chemistry.reactions       = [
  # totally diffusion-controlled (TDC)
  [["H", "H"], ["H2"], "Fix", 0.5e10, 0],
  [["e_aq", "H"], ["H2", "OHm"], "Fix", 2.5e10, 0],
  [["e_aq", "e_aq"], ["H2", "OHm", "OHm"], "Fix", 0.636e10, 0],
  # partially diffusion-controlled (PDC)
  [["OH", "H"], ["H2O"], "Fix", 1.55e10, 1],
  # ...
]
```

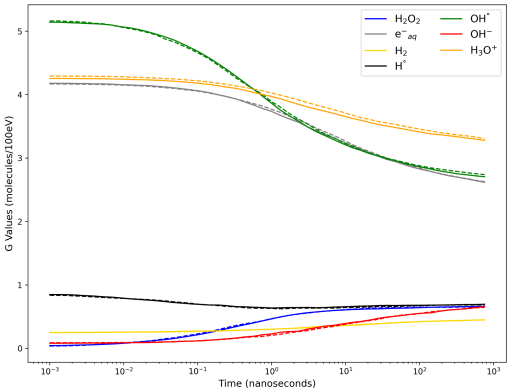
Chemistry actor – output – work in progress

```
chemistry.get_times()
# [0.001, ..., 754.311, 999.999]

chemistry.get_data_v()  # species count, G values, ...
# {
#  'H2O2^0': {'count': [...]}, 'g': [...]},
#  ...,
# }

chemistry.get_reactions()  # all reactions by time
# {
#  0.001: [{'reactants': ['OH^-1', 'ºOH^0'], 'products': ['O^-1']}, ...]
#  ...,
# }
```

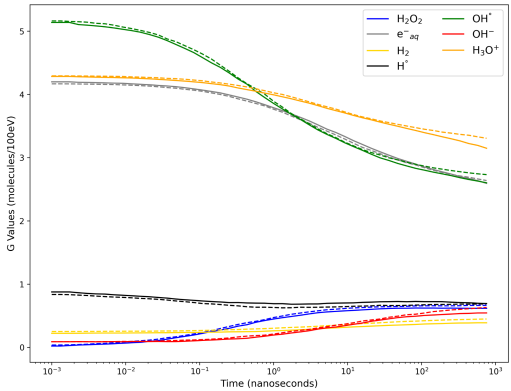
Chemistry actor – results

Geant4-DNA (chem6) dashed; GATE 10 plain

IRT (Independent Reaction Time)



SBS (Step by Step)



Simulation and analysis by Da Eun Kwon

Conclusion

BioDose actor

- available in current GATE release (9.4.1)
- work in progress version in GATE 10 (branch `biodoseactor`)
- paper in preparation

Chemistry actor

- work in progress version in GATE 10 (branch `dnachemistry`)
- ongoing validation for UHDR ion beam lines

Thank you for your attention