

# BioDose and Chemistry actors in GATE 10

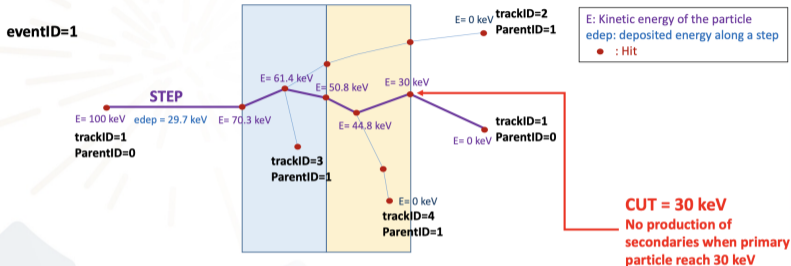
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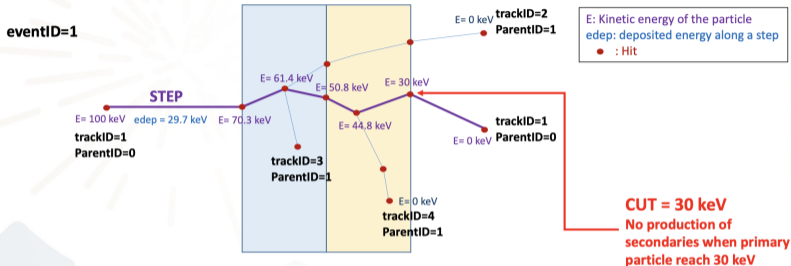
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AG GdR Mi2B 2024



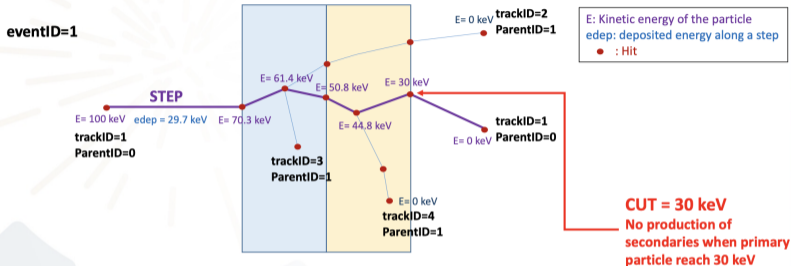
## Geant4 actions

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



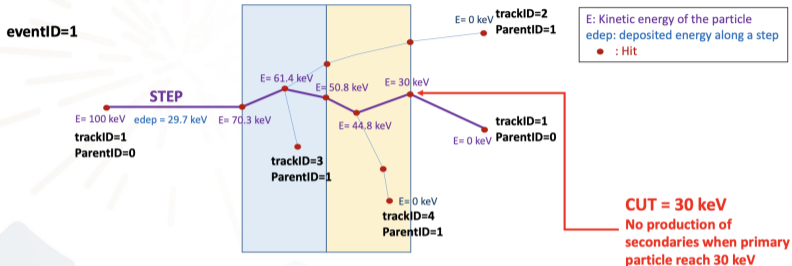
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compute biodose	✓	✓	✓	✓	✓	
apply chemistry				✓	✓	✓



## Geant4 actions

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



## Geant4 actions

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

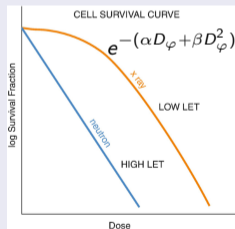
## Objective of the biological dose

effects of the physical dose on biological tissues

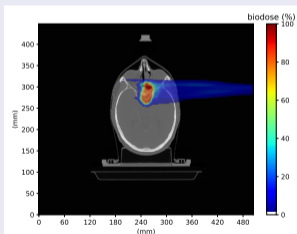
### nano/micro scale

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

### cellular scale



### macro scale



Cell line Human Salivary Glands (HSG): HSG\_mMKM.db or HSG\_NanOx.db

⇒ easy to provide new cell lines or biophysical models

Example:

$\alpha, \beta$ : from Geant4-DNA/LPCHEM simulations

```
// Ion type
```

```
H
```

```
...
```

```
He
```

```
...
```

```
C
```

```
...
```

```
O
```

```
...
```

```
Li
```

```
...
```

```
// energy
```

```
// (MeV)
```

```
alpha
```

```
(Gy-1)
```

```
beta
```

```
(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
```

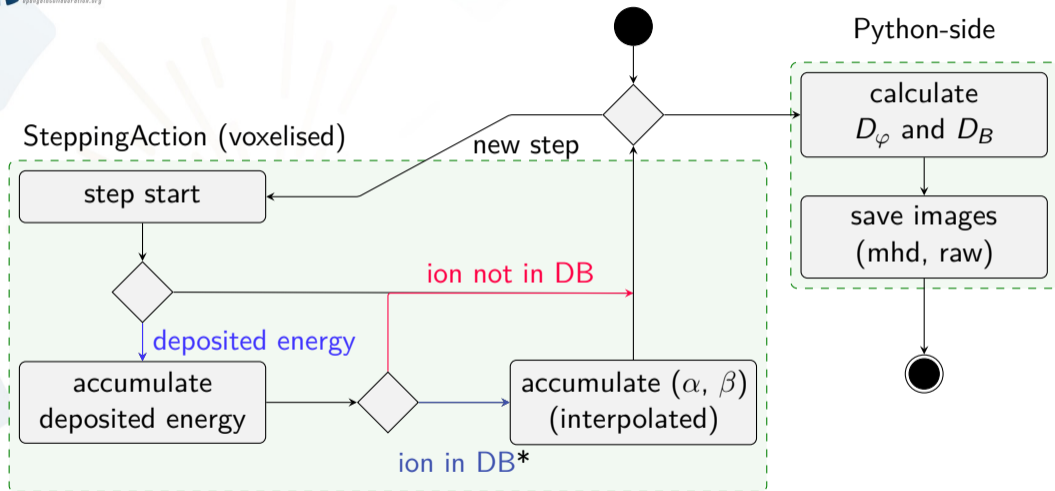
```
...
```

```
300
```

```
0.339
```

```
0.109
```

# BioDoseActor process diagram



\* our database (DB) contains values for {H, He, C, O, Li}

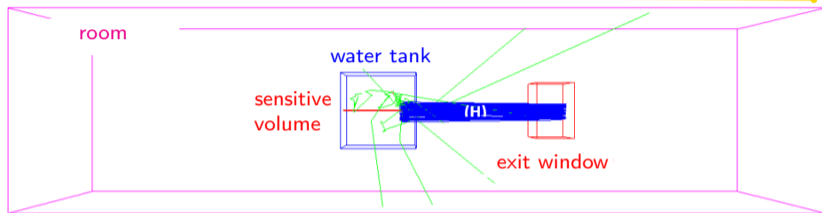


```
biodose = sim.add_actor("BioDoseActor", "biodose")

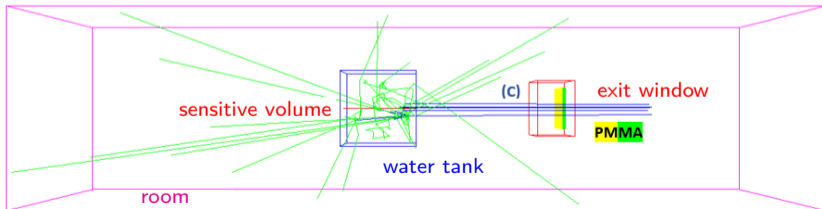
biodose.attached_to      = volume
biodose.output_filename = "biodose.mhd"
biodose.translation     = [0, 0, 0]
biodose.spacing         = [1 * mm, 60 * mm, 60 * mm]
biodose.size            = [400, 1, 1]

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

H-ion:

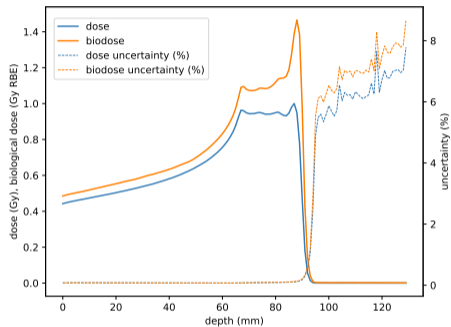


C-ion:

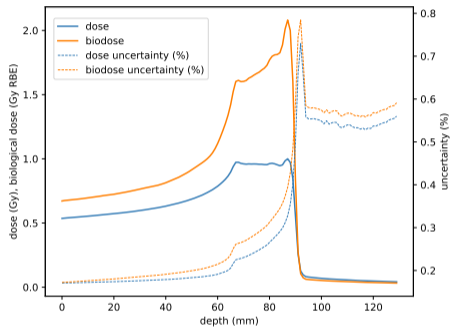


- Human Salivary Glands
- Pencil Beam Scanning:
  - H: 95.9 – 113 MeV
  - C: 120 – 402 MeV/u
- Water box:  
400 × 400 × 400 mm<sup>3</sup>
- Sensitive volume:  
400 × 60 × 60 mm<sup>3</sup>
- Voxel size:  
1 × 60 × 60 mm<sup>3</sup>
- PhysicsList:
  - H: QGSP\_BIC\_EMZ
  - C: Shielding\_EMZ
- multiple stepfunctions
- multiple steplimiters

## Results – dose profiles

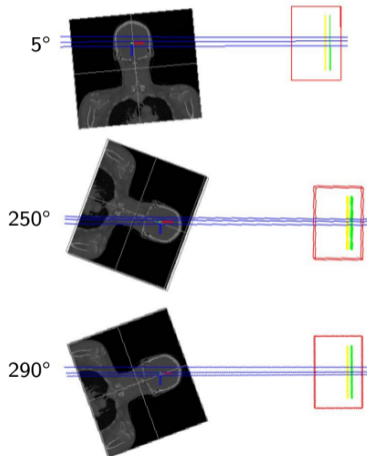


**Figure:** H-ion in water with  $1 \times 10^7$  primaries, production cut 100 m, step limiter 10  $\mu\text{m}$  (HSG, NanOx)

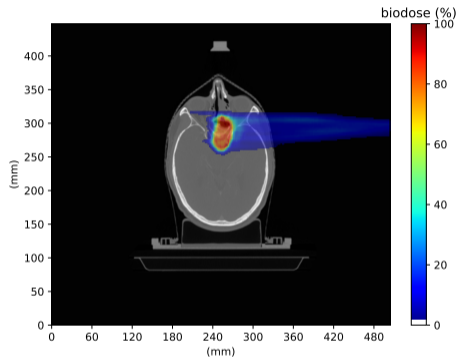


**Figure:** C-ion in water with  $1 \times 10^6$  primaries, production cut 100 m, step limiter 10  $\mu\text{m}$  (HSG, mMKM)

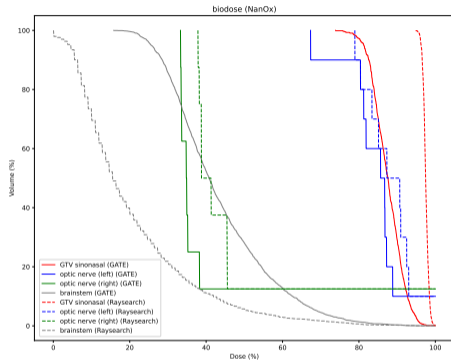
- Human Salivary Glands
- Pencil Beam Scanning
- CT:  $50 \times 50 \times 44 \text{ cm}^3$
- Voxel size:  
 $0.97 \times 0.97 \times 2 \text{ mm}^3$
- PhysicsList:  
 Shielding\_EMZ
- 3 beams
- sinonasal chordoma



## Results – C-ion, biological dose (NanOx)



**Figure:** biological dose with C-ion in patient,  $1 \times 10^6$  primaries per beam, production cut 100 m, step limiter  $10 \mu\text{m}$  (HSG, NanOx)



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

# Chemistry actor

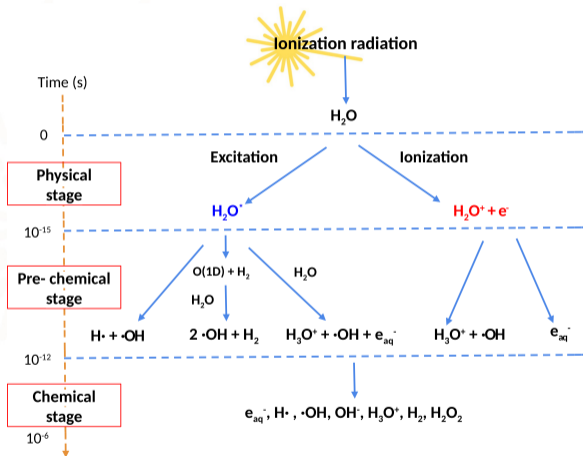


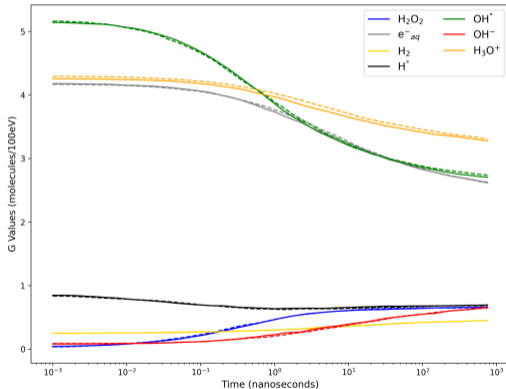
Figure from Da Eun Kwon

```
chemistry = sim.add_actor("ChemistryActor", "chemistry")
chemistry.attached_to      = volume
chemistry.timestep_model  = "IRT" # or "SBS"
chemistry.end_time        = 1 * ns
chemistry.time_bins_count = 50
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}],
    [{"H3Op", "OHm"}, {"H2O"}, {"Fix", 1.13e11, 0}],
    # partially diffusion-controlled (PDC)
    [{"OH", "H"}, {"H2O"}, {"Fix", 1.55e10, 1}],
    # ...
]
```

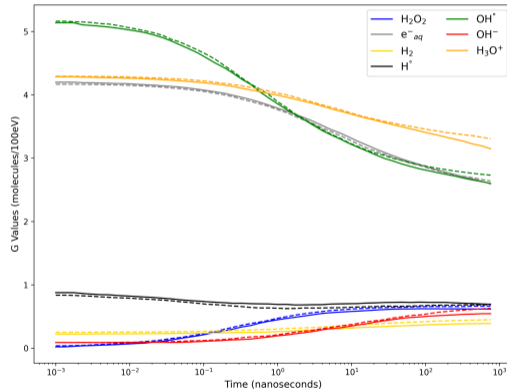
# Chemistry actor – results

Geant4-DNA (chem6) dashed; GATE 10 plain

## IRT (Independent Reaction Time)



## SBS (Step by Step)



Simulation and analysis by Da Eun Kwon



### BioDose actor

- available in current GATE release (9.4)
- will be available with next GATE release (10)

### Chemistry actor

- still work in progress
- first version for end of 2024