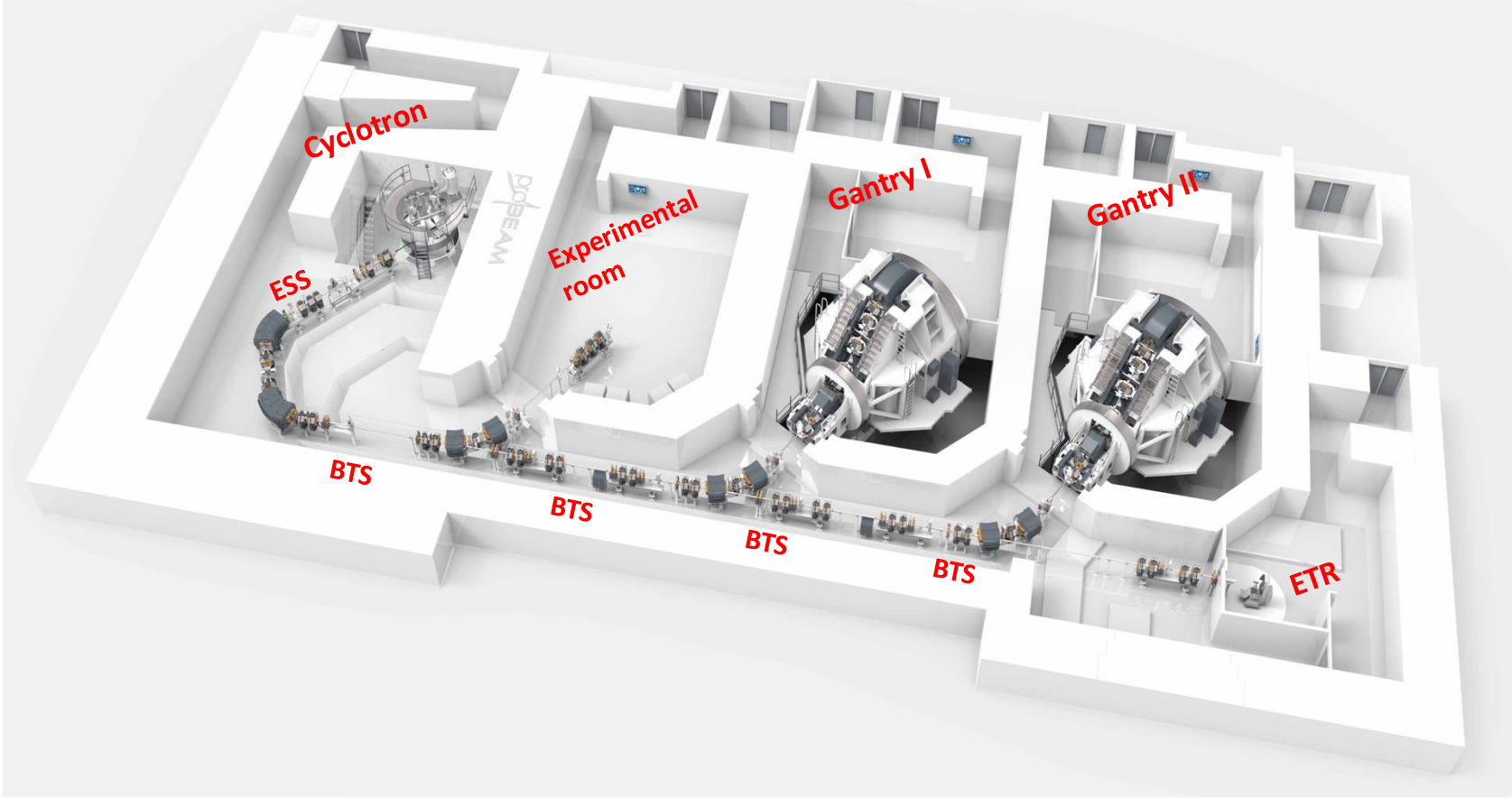
Towards Geant4-DNA in GATE 10

GATE Scientific meeting 2026, Strasbourg

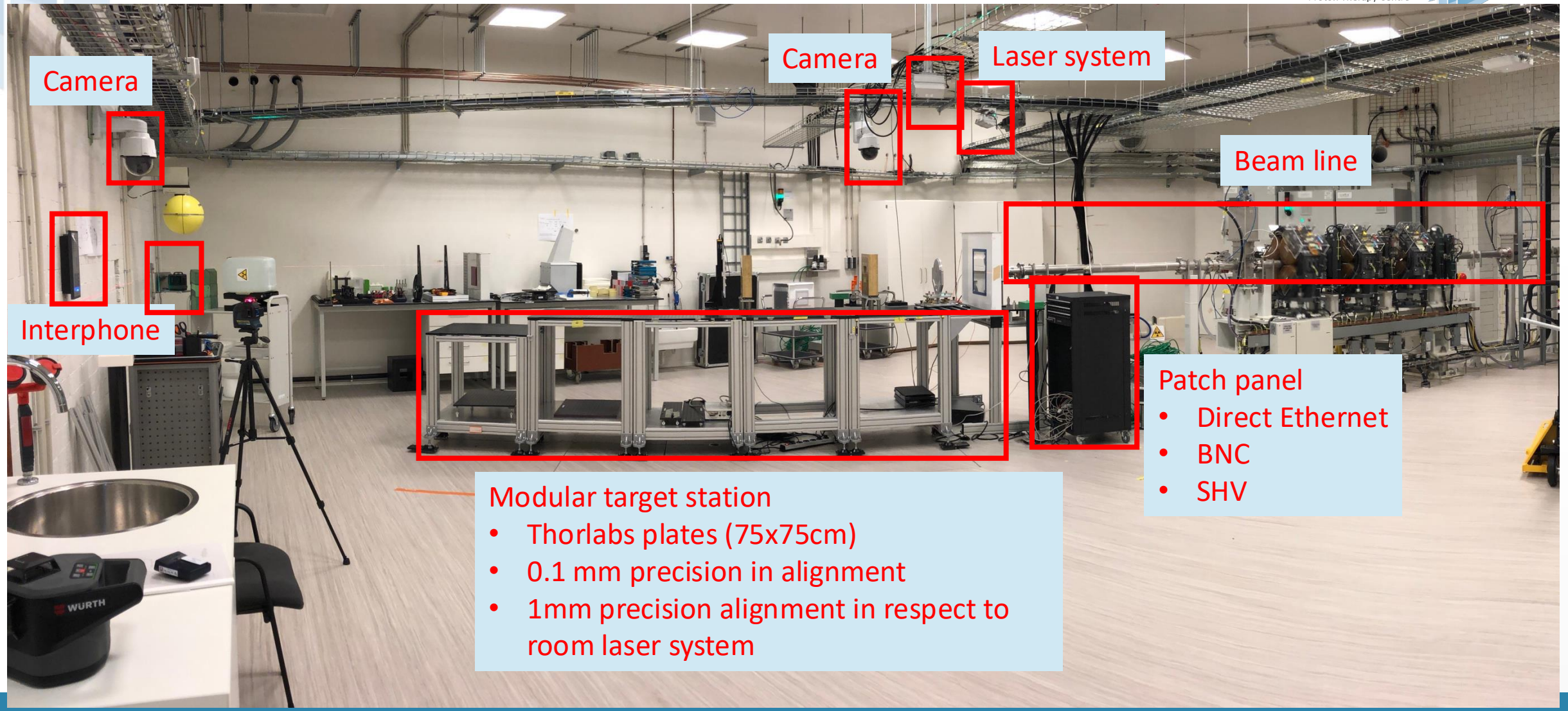
Nils Krah, April 1, 2026

The Holland Proton Therapy Center

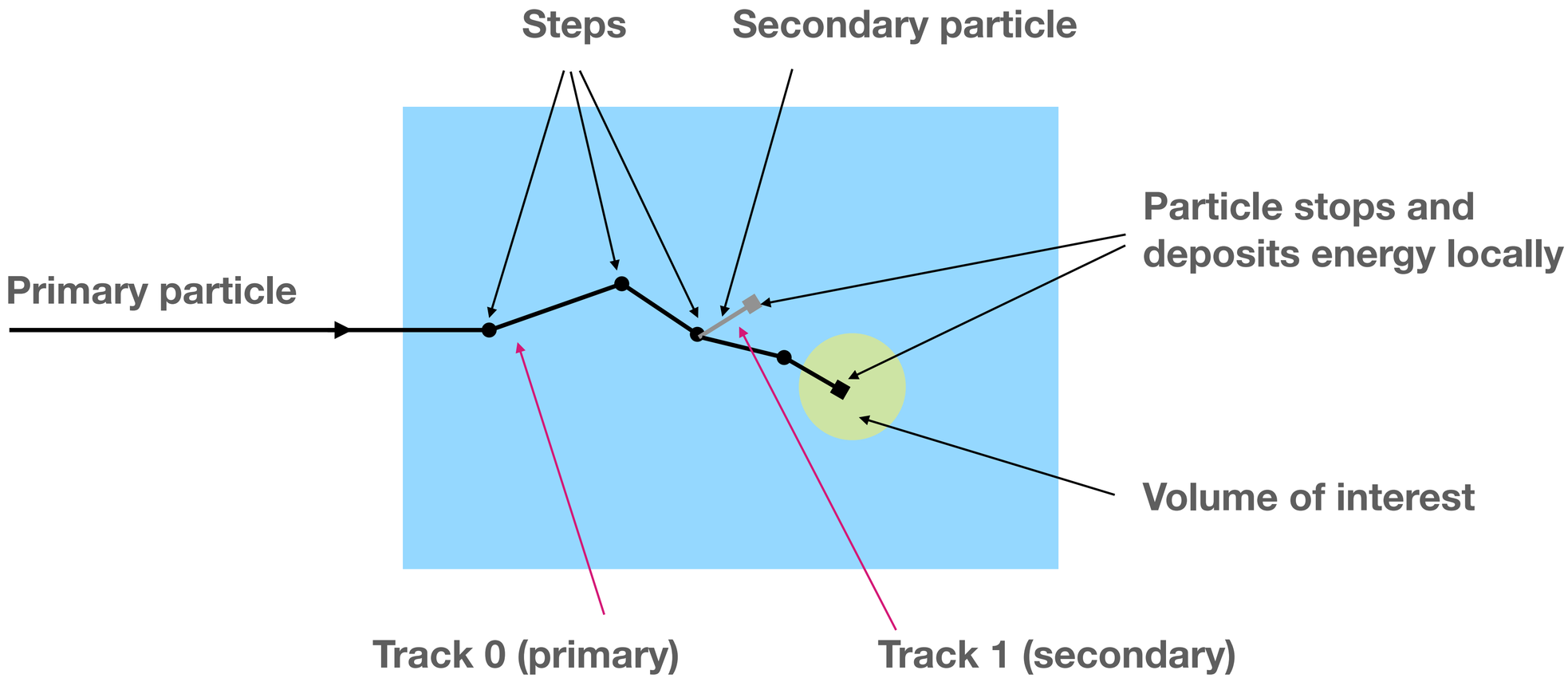
- VARIAN Protontherapy Center
- Superconductive Cyclotron ProBeam
- 4 rooms:
  - 2 rotating gantries,
  - 1 eye treatment room
  - 1 R&D room



The experimental room



Reminder: Step-wise transport in Geant4

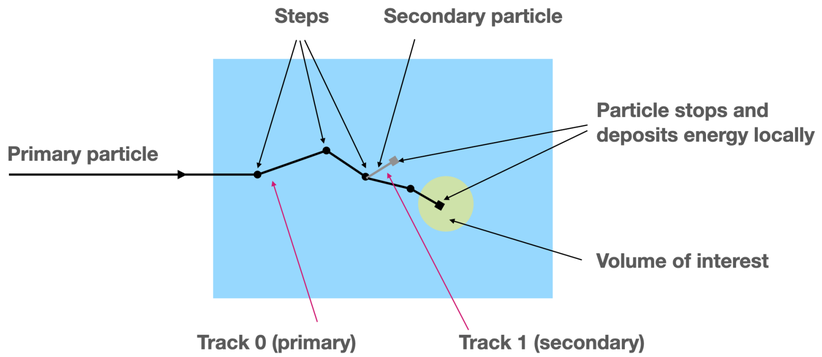


Geant4 *always* uses variance reduction technique.

… really?

Condensed history simulation = VRT

- Geant4 does **not** simulate each real interaction explicit
- Instead: simulate the effective result of interactions condensed into a finite sized step
- Step length is dynamic: depends on the processes, material, and particle
- Advantage: makes computation speed bearable
- Disadvantage: cannot “resolve” physics below on smaller scale than step length



Why would we need a simulation on smaller scales?

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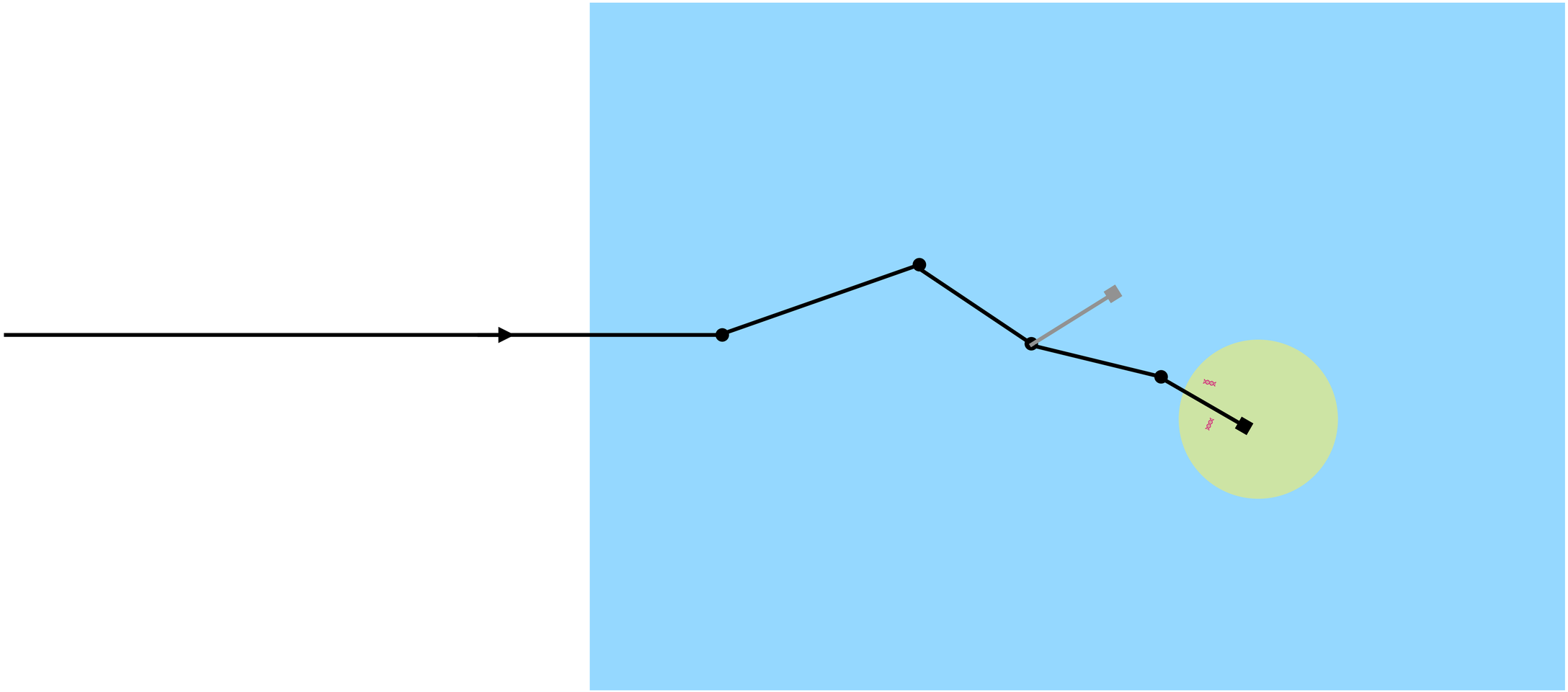
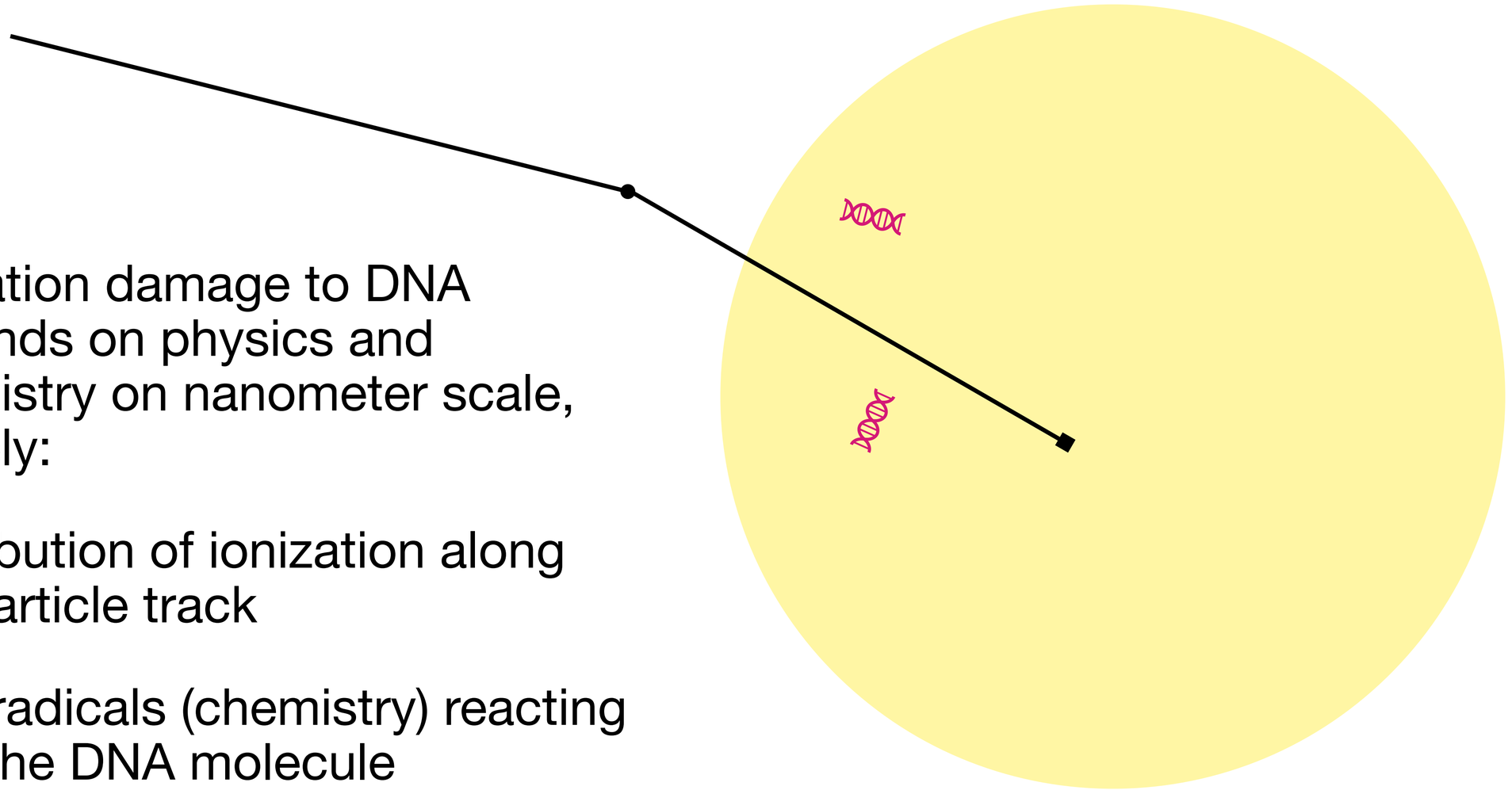


DNA is on nanometer scale



- Radiation damage to DNA depends on physics and chemistry on nanometer scale, namely:
- Distribution of ionization along the particle track
- Free radicals (chemistry) reacting with the DNA molecule

Geant4-DNA

- Geant4-DNA is part of Geant4
- Provides EM physics processes down to eV energy level
- Adds a chemical stage which simulates diffusion and reactions
- Tiny steps means slow simulation -> only in small selected volumes
- GATE does not leverage Geant4-DNA … yet

Integrating Geant4-DNA in GATE 10

Two main challenges:

1. Make Geant4-DNA EM physics selectable per (small) volume
2. Integrate the chemistry simulation stage

The work I show is in PR #976:

https://github.com/OpenGATE/opengate/pull/976

Make Geant4-DNA EM physics selectable per volume

User should be able to do this:

```
    sim.physics_manager.physics_list_name = "G4EmStandardPhysics"
    target = sim.add_volume("Box", "chem_box")
    target.size = [10 * um, 10 * um, 10 * um]
    target.material = "G4_WATER"
    target.set_dna_em_physics("DNA_Opt2")
```

… to select G4EmDNAPhysics_option2 in the target instead of G4EmStandardPhysics

DNA EM physics selectable per volume

- Leverage the Region concept, i.e. logical groups of volumes
- target.set_dna_em_physics(“DNA_Opt2”) -> GATE creates a Region and associates the volume “target” with it
- Region holds info about DNA Em Physics
- Consider region-wise physics during initialization

Region DNA EM physics - initialization

During initialization (SimulationEngine.initialize()), GATE now does:

1. Check if any region exists that requests DNA Em physics
2. If so, create G4EmDNAPhysicsActivator and register it to physics list
3. For all regions that request DNA Em Physics, communicate this couple to G4EmParameters:

   g4_em_parameters.AddDNA(region.name, region.dna_em_physics)

4. Adapted initialization sequence for Geant4 compatibility

Actors can request DNA EM physics

During initialization (SimulationEngine.initialize()), GATE now does:

1. FancyActor.dna_em_physics defines the DNA Em physics needed by the actor

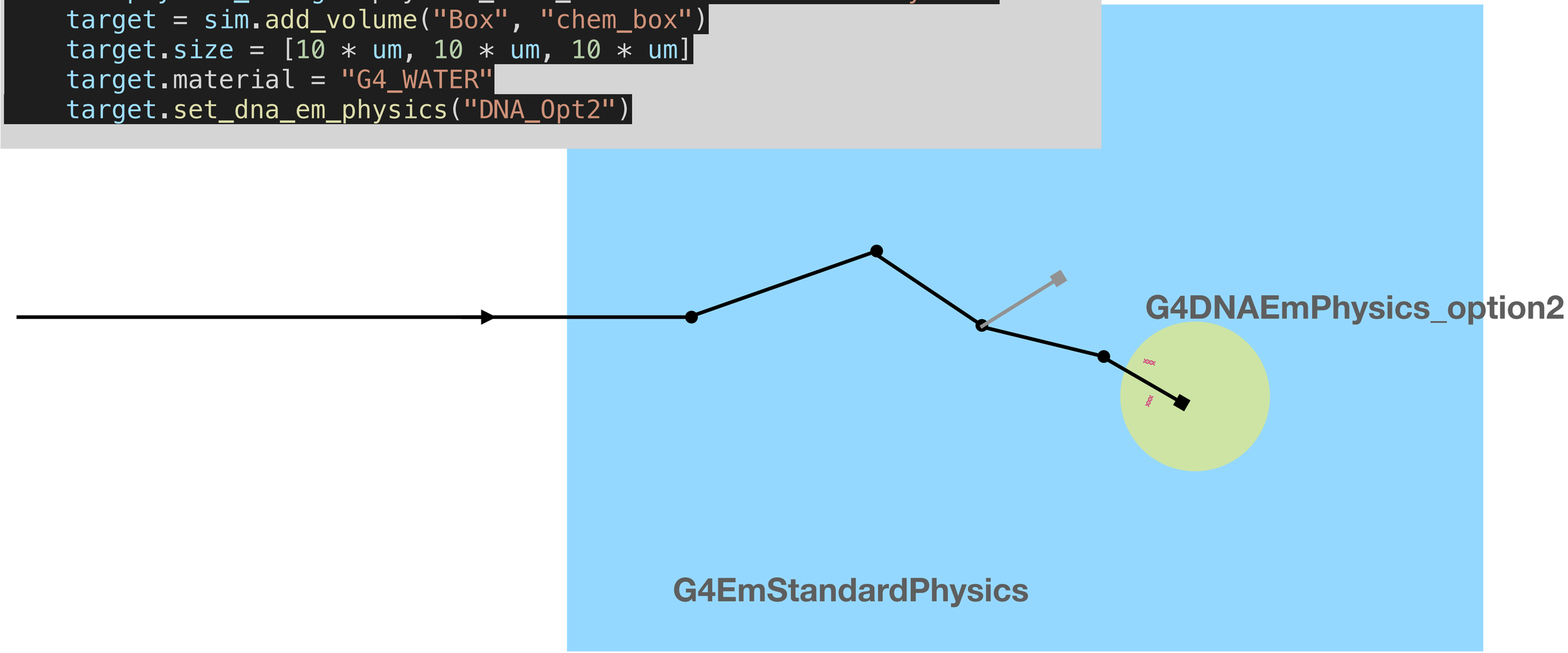
2. At the beginning of initialization, GATE checks to which volume the actor is attached

3. Check for conflicting DNA Em Physics requests

4. Create region and set dna_em_physics for the volume to which the actor is attached

Tiny eV scale simulation in sub volume

```
    sim.physics_manager.physics_list_name = "G4EmStandardPhysics"
    target = sim.add_volume("Box", "chem_box")
    target.size = [10 * um, 10 * um, 10 * um]
    target.material = "G4_WATER"
    target.set_dna_em_physics("DNA_Opt2")
```



Integrating Geant4-DNA in GATE 10

Two main challenges:

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Reminder: Geant4 event loop

- Begin new event (new primary) and generate primary track
- Step-wise transport of this track
- Secondaries particles -> new tracks: collected on a stack
- Once current track done -> continue with next track from the stack
- No tracks left -> move to new event (primary)

Rationale Chemistry simulation

- Chemistry takes place at low energy
- At the end of a track (low particle energy), start chemical simulation stage
- Important: chemical simulation moves forward in time steps
- Reason: Chemical reactions take place at different speeds
- Another reason: diffusion and Brownian motion are better described in time-domain

GATE must handle chemistry list and trigger chemistry simulation

How is chemistry connected with GATE10/Geant4-DNA?

- Processes in DNA-EmPhysics create chemical species (molecules) relevant for reactions
- Turn them into tracks and “tag” them as relevant for chemistry
- When no standard tracks are left on the stack, GATE triggers G4DNAChemistryManager::Instance()->Run();
- This triggers the G4Scheduler that handles the time-stepping

Chemisty Actors

- GATE now has a new sub-class of actors
- Intermediate base classes
  - Python: ChemistryActorBase
  - C++: GateVChemistryActor
- The actor can request a certain chemistry list
- And implement chemistry actions

Chemistry Actor actions

Chemistry actions are:

- GateVChemistryActor
- StartChemistryTracking(G4Track*)
- EndChemistryTracking(G4Track*)
- BeginOfChemicalStage()
- EndOfChemicalStage()
- UserPreTimeStepAction()
- UserPostTimeStepAction()
- UserReactionAction(const G4Track&, const G4Track&, const std::vector<G4Track*>*)

Example: ChemicalStageActor

Derived from Geant4-DNA chem6 example

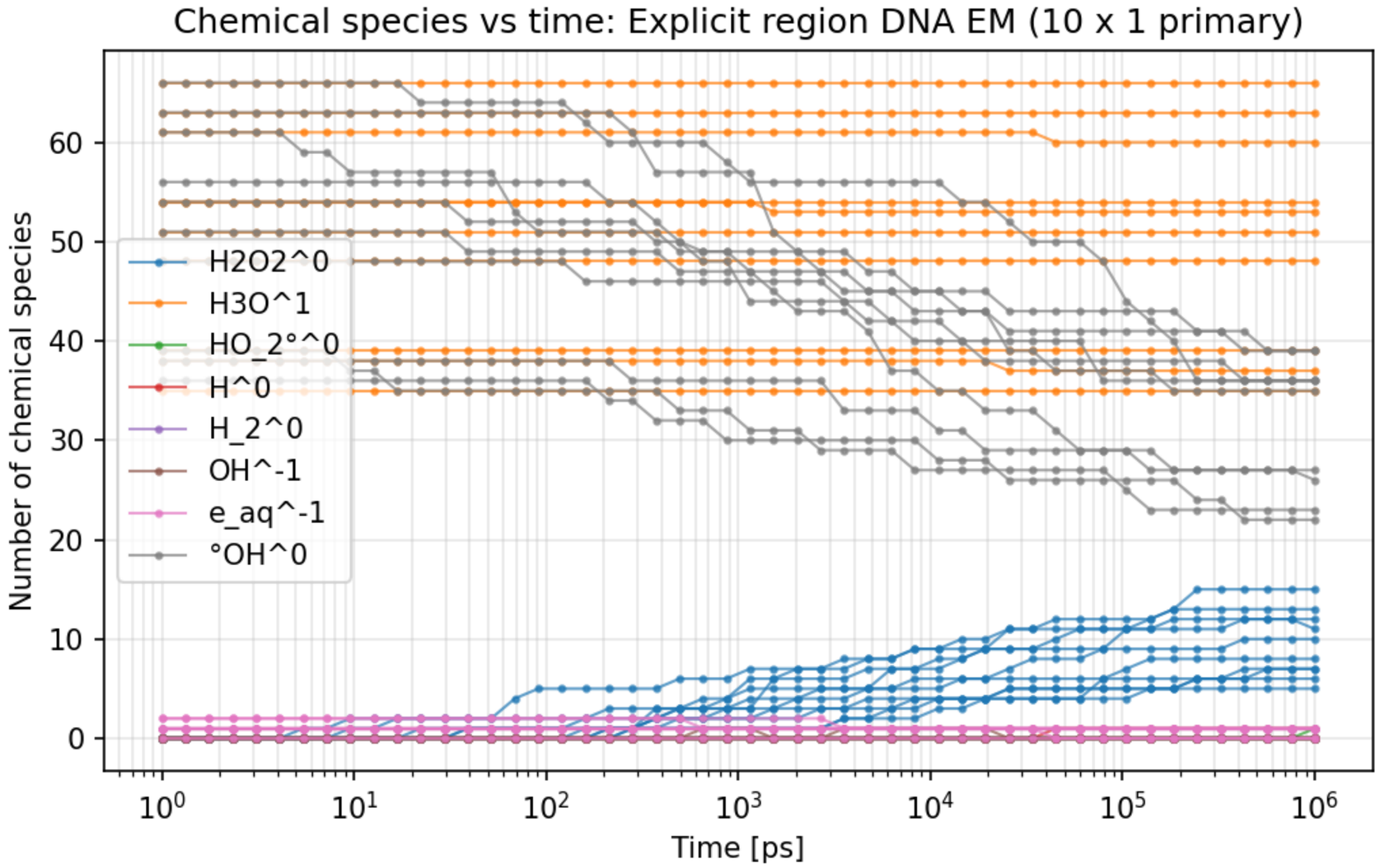
- Keeps statistics of chemical species created during chemistry simulation (when, what)
- Implements UserReactionAction()

```
    chem_actor = sim.add_actor("ChemicalStageActor", "chem_actor")
    chem_actor.attached_to = target
    chem_actor.number_of_time_bins = 50
    chem_actor.dna_em_physics = "DNA_Opt2"
```

Example: ChemicalStageActor

- electron with 2 keV in a water phantom 10x10x10 um^2
- Overall physics: G4EmStandardPhysics
- In phantom: G4EmDNAPhysics_option2 and G4EmDNAChemistry_option3

Example: ChemicalStageActor



Summary

- GATE 10 can now handle DNA Em physics, per volume
- Physics simulation down to eV level possible
- Example: track structure simulation possible
- Chemistry architecture working, but some bugs to be fixed
- First Chemistry actor implemented

To-Do

- Chemistry-equivalent to digi attributes
- Data structure for chemistry “digs attributes”
- Filters for chemistry stage
- Implement meaningful ChemistryActors -> contributions welcome

Thanks