Flagged uniform particle split for Geant4-DNA

José Ramos-Méndez and Bruce Faddegon.

Department of Radiation Oncology
UCSF Helen Diller Family Comprehensive Cancer Center

21st Geant4 Collaboration meeting, 2016
Outline

• Brief review to the variance reduction in radiotherapy
• Flagged uniform particle split
• Computational efficiency and accuracy
• Use cases
• Conclusions

Flagged uniform particle split for Geant4-DNA
Variance reduction in radiotherapy

Enhance the computational efficiency by using: Variance reduction or Approximate efficiency improvement techniques:

- Physical models
- Truncation methods
- Population control methods

\[ \sigma \leftarrow f\sigma \]

Flagged uniform particle split for Geant4-DNA
Variance reduction in radiotherapy

Particle splitting is the most popular variance reduction in radiotherapy. Flagged uniform particle split for Geant4-DNA.

Applied at specific physical process.

Geometrical Interface
Variance reduction in radiotherapy

Particle splitting is the most popular variance reduction in radiotherapy.

Flagged uniform particle split for Geant4-DNA.
Variance reduction in radiotherapy

Particle splitting is the most popular variance reduction in radiotherapy.

Flagged uniform particle split for Geant4-DNA

Geometrical

Applied at specific physical process

10 bp
~3.4 nm

Flagged uniform particle split for Geant4-DNA
Variance reduction in radiotherapy

Particle splitting is the most popular variance reduction in radiotherapy.

Flagged uniform particle split for Geant4-DNA

10 bp ~3.4 nm

Applied at specific physical process

After particle splitting
Flagged uniform particle split

A unique flag (integer) is used to keep track of each new split particle

- This flag must be **inherited** to all subsequent secondaries
- Use this flag to classify all the tracks independently
- A similar method to Get/SetWeight was implemented to allow the propagation of the flag to the secondary particles

Flagged uniform particle split for Geant4-DNA
Flagged uniform particle split

- A unique flag (integer) is used to keep track of each new split particle
- This flag must be **inherited** to all subsequent secondaries
- Use this flag to classify all the tracks independently
- A similar method to Get/SetWeight was implemented to allow the propagation of the flag to the secondary particles

Split $N_s=3$

Flagged uniform particle split for Geant4-DNA
Flagged uniform particle split

A unique flag (integer) is used to keep track of each new split particle

- This flag must be **inherited** to all subsequent secondaries
- Use this flag to classify all the tracks independently
- A similar method to Get/SetWeight was implemented to allow the propagation of the flag to the secondary particles

Split $N_s = 3$

Flagged uniform particle split for Geant4-DNA
Flagged uniform particle split

- The split process was implemented by means of the G4WrapperProcess

```cpp
newSplitID = 3;
For i=1 to numberOfSplit
    newTrack = new G4Track(*(particleChange->GetSecondary(j)))
    newWeight = w0/numberOfSplit
    newSplitID += 1
    ...
If particle is an electron
    particleChange->ProposeSplitTrackID(2)
    particleChange->SetSecondaryWeightByProcess(true)
    particleChange->SetSecondarySplitTrackIDByProcess(true)
    ...
... In UserWrappedProcess() Apply to X_G4DNAIonisation()
```
Flagged uniform particle split

- The split process was implemented by means of the G4WrapperProcess

... newSplitID = 3;
For i=1 to numberOfSplit
    newTrack = new G4Track(*(particleChange->GetSecondary(j)))
    newWeight = w0/numberOfSplit
    newSplitID += 1
...

If particle is an electron
    particleChange->ProposeSplitTrackID(2)
particleChange->SetSecondaryWeightByProcess(true)
particleChange->SetSecondarySplitTrackIDByProcess(true)

In UserWrappedProcess()
    Apply to X_G4DNAIonisation()

In ProcessHits()

    // In constructor
    For i=1 to numberOfSplit
        fMyScorer[i] = CreateCopyScorer(i);
    // In ProcessHits
    splitID = aStep>GetPreStepPoint()->GetSplitTrackID(); // or from preStepPoint
    weight = aStep->GetPreStepPoint()->GetWeight();
    if splitID > 2
        fMyScorer[splitID-3]->Accumulate(position, edep*weight, etc);
    else
        for i=1 to numberOfSplit
            fMyScorer[i]->Accumulate(position, edep*weight, etc);

    // After simulation
    Normalize Final Distribution to numberOfSplit.
Computational efficiency and accuracy

Computational efficiency

The computational efficiency $\varepsilon$ of a Monte Carlo simulation, that takes the execution time $T$ to recover the quantity of interest $X$, with variance $\sigma^2$ is given by

$$\varepsilon = \frac{1}{\sigma^2 T}$$

Scoring metric

Two meaningful quantities of interest in nanodosimetry are the first moment $M_1(Q)$ and the cumulative distribution $F_2(Q)$ of the ionization distribution $P(\nu|Q)$ produced by a particle beam of quality $Q$ \(^a\); where the cluster size $\nu$ is defined as the number of ionizations produced within the scoring region by a single history

$$M_1(Q) = \sum_{\nu=0}^{\infty} \nu P(\nu|Q) \quad F_2(Q) = \sum_{\nu=2}^{\infty} P(\nu|Q)$$

**Use cases** (Geant4.10.2.p02)

- Cylindrical target of 6 nm diameter and 10 nm length embedded into a cubic box (World) of 150 nm side \(^{a}\).
- The number of ionizations per history inside the target was scored.

---

Use cases

- Cylindrical target of 6 nm diameter and 10 nm length embedded into a cubic box (World) of 150 nm side [a].
- The number of ionizations per history inside the target was scored.

- Box target of 0.5 μm thickness and 1 μm length embedded into a cubic box (World) of 2 μm side.
- DBSCAN parameters: 3.2 nm, $E_{\text{min}}=5$ eV, $E_{\text{max}}=35$ eV, probability of 16% [b].
- The number of SSB and DSB per history inside the target was scored.

---


**Use cases**

- Ionization distributions

  - Cylindrical target of 6 nm diameter and 10 nm length embedded into a cubic box (World) of 150 nm side \(^a\).
  - The number of ionizations per history inside the target was scored.

  - Box target of 0.5 μm thickness and 1 μm length embedded into a cubic box (World) of 2 μm side.
  - DBSCAN parameters: 3.2 nm, \(E_{\text{min}}=5\) eV, \(E_{\text{max}}=35\) eV, probability of 16% \(^b\).
  - The number of SSB and DSB per history inside the target was scored.

- Clustering: Single and Double DNA strand breaks with DBSCAN

  - Box target of 9.71 x 7.61 x 12.63 nm\(^3\) embedded into a cubic box of 100 nm side.
  - The coordinates of the atoms (Protein Data Bank format) are used to define if an ionization event is taken into account. If the ionization event (\(E > 8.22\) eV) is within a distance lower than the Van der Waals radius from an atom, then it is scored \(^c\).
  - A double strand breaks occurs if two single strand breaks occur in opposite strands within 10 base pairs.

  In all cases, the source was mono energetic carbon ions or protons of 1-20 MeV/u or 0.5-20 MeV, respectively.

---


Results: protons

Top: Relative efficiency versus the number of split $N_s$ for several energies of the incoming proton source. Error bars represent statistical uncertainty at one standard deviation.

Flagged uniform particle split for Geant4-DNA
Results: protons

**Top:** Relative efficiency versus the number of split $N_s$ for several energies of the incoming proton source. Error bars represent statistical uncertainty at one standard deviation.

**Bottom:** First moment $M_1(Q)$ and cumulative distribution $F_2(Q)$ of $P(v|Q)$ in function of the kinetic energy of the proton for the two physical process improved with the flagged uniform particle split. In both cases, on the right axis is shown the relative difference (filled markers) with respect to reference data (without flagged particle split) in percent. The error bars (in some cases smaller than the markers) represent one standard deviation.

Flagged uniform particle split for Geant4-DNA
Results: Carbon ions

Left: Relative efficiency versus the number of split $N_s$ for several energies of the incoming carbon ion source. The flagged uniform particle split was applied to the process $\text{e-}_\text{G4DNAIonisation}$. Right: Cluster size probability distributions for several energies for the reference simulation (markers) and the variance-reduced simulations (solid lines). The inset shows the fractional uncertainty in percent for the probability distribution corresponding to carbon ions of 1 MeV/u. The error bars represent one standard deviation.

Flagged uniform particle split for Geant4-DNA
**Results: DBSCAN**

Top: Relative efficiency versus the number of split $N_s$ for several energies of the incoming proton (left) and carbon ion (right) source. The error bars represent one standard deviation.

Flagged uniform particle split for Geant4-DNA
Results: DBSCAN

**Top:** Relative efficiency versus the number of split $N_s$ for several energies of the incoming proton (left) and carbon ion (right) source. The error bars represent one standard deviation.

**Bottom:** The mean number of DBS and SSB for proton energies from 0.5 to 50 MeV and carbon ions from 1 to 20 MeV/u are shown. Lines are for guide the eyes. The flagged uniform particle split was applied with $N_s=64$ for protons and $N_s=32$ for carbon ions. The relative difference in percent is shown on the right axis.

Flagged uniform particle split for Geant4-DNA
Results: PDB4DNA

Top: Relative efficiency versus the number of split \(N_s\) for several energies of the incoming proton (left) and carbon ion (right) source. The error bars represent one standard deviation.
Results: PDB4DNA

Top: Relative efficiency versus the number of split $N_s$ for several energies of the incoming proton (left) and carbon ion (right) source. The error bars represent one standard deviation.

Bottom: The mean number of DBS and mean SSB for proton energies from 0.5 to 50 MeV and carbon ions from 1 to 20 MeV/u are shown. Lines are for guide the eyes. The flagged uniform particle split was applied with $N_s=256$ for protons and $N_s=512$ for carbon ions. The relative difference in percent is shown on the right axis.

Flagged uniform particle split for Geant4-DNA
Conclusions

• 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. The efficiency improvement depended on the complexity of the scoring of the quantity of interest, and the LET of the particle of interest, being larger for low LET particles and less complex scoring methods.

• For protons, the efficiency ranged from about a factor of 7 to 20 (for complex scoring, high to low LET) to about 50 to 350 (less complex scoring, high to low LET). For carbon ions, the efficiency ranged from about a factor of 4.5 to 5 (for complex scoring, high to low LET) to 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.