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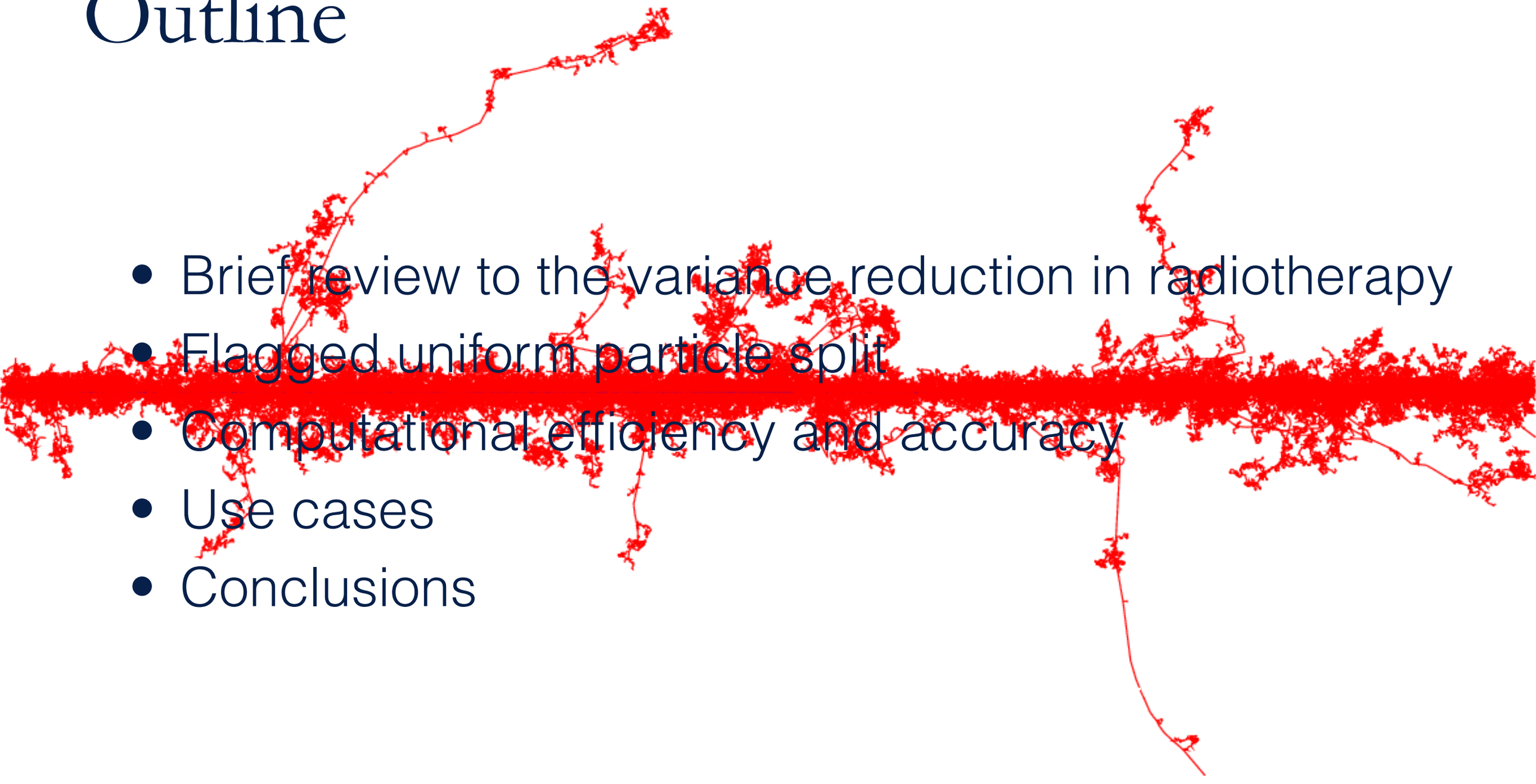
Flagged uniform particle split for Geant4-DNA

José Ramos-Méndez and Bruce Faddegon.

Department of Radiation Oncology
UCSF Helen Diller Family Comprehensive Cancer Center

21st Geant4 Collaboration meeting, 2016

Outline

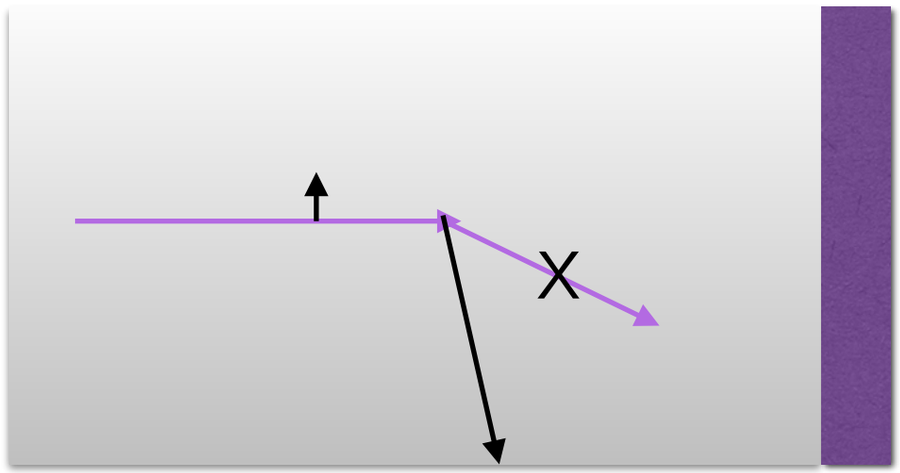


- Brief review to the variance reduction in radiotherapy
- Flagged uniform particle split
- Computational efficiency and accuracy
- Use cases
- Conclusions

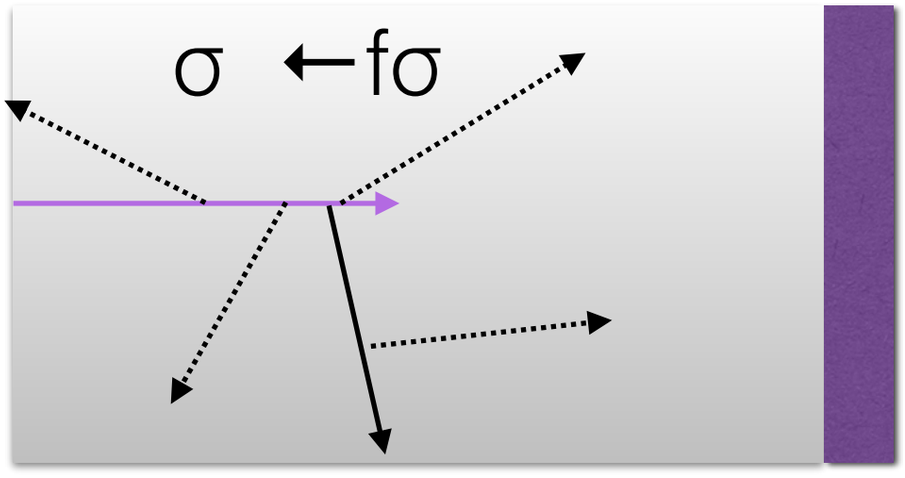
Variance reduction in radiotherapy

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

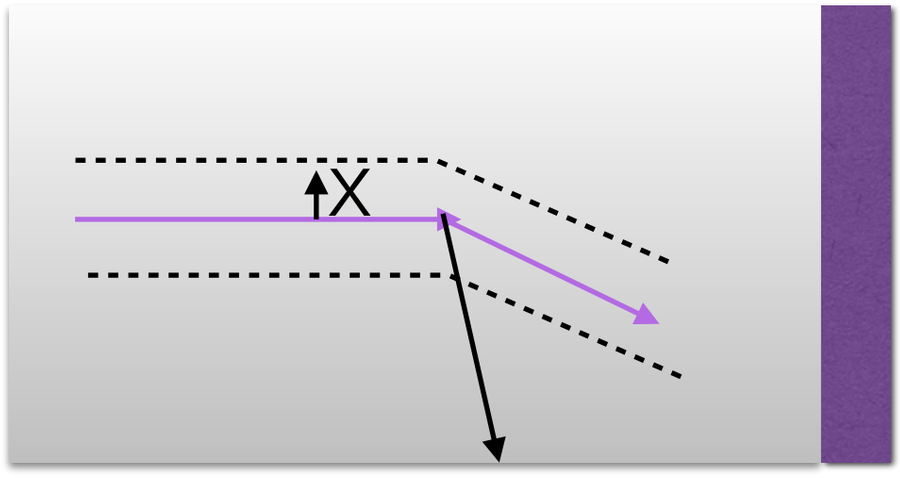
- Physical models
- Truncation methods
- Population control methods



Range rejection



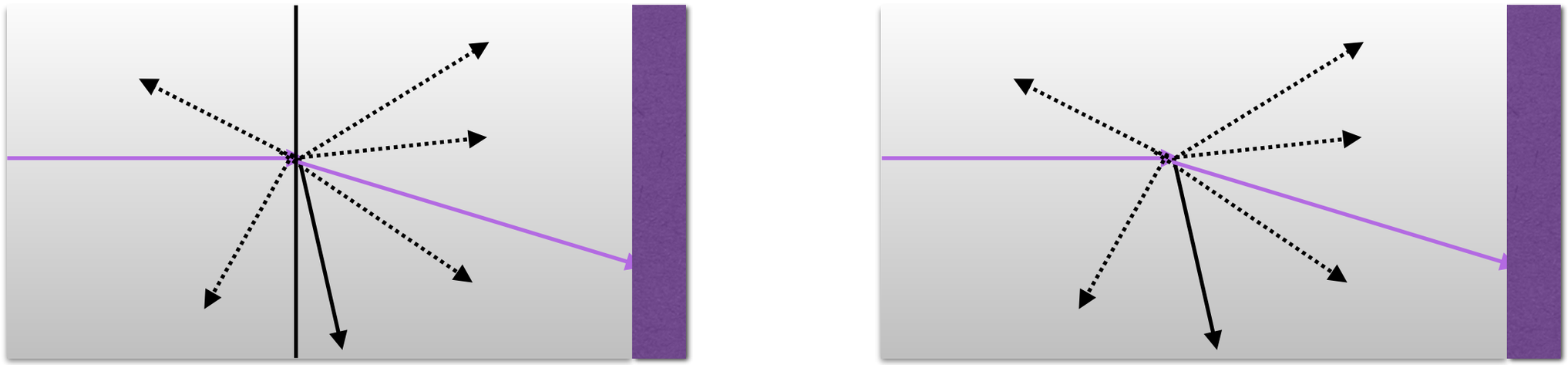
Cross-section enhancement



Production cuts

Variance reduction in radiotherapy

Particle splitting is the most popular variance reduction in **radiotherapy**



Geometrical

Applied at specific physical process

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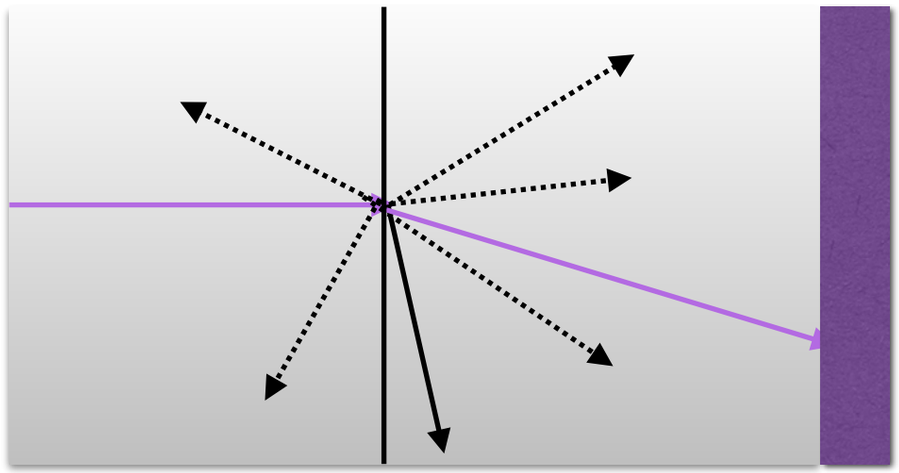
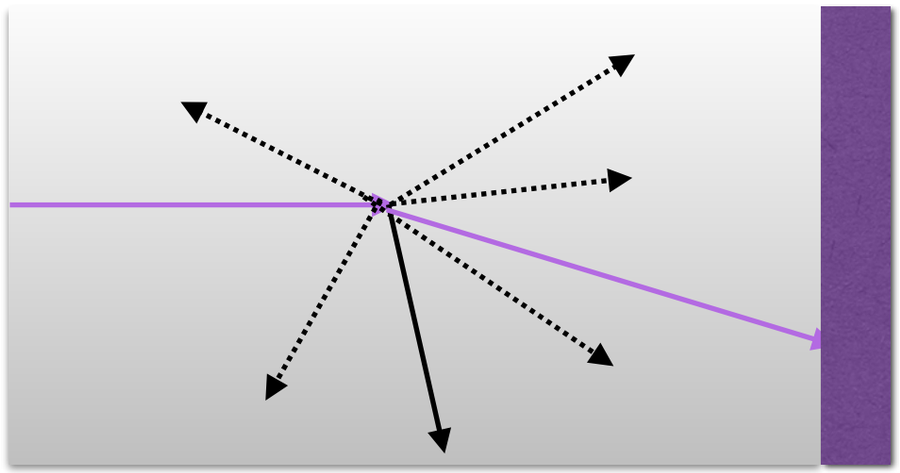


Geometrical



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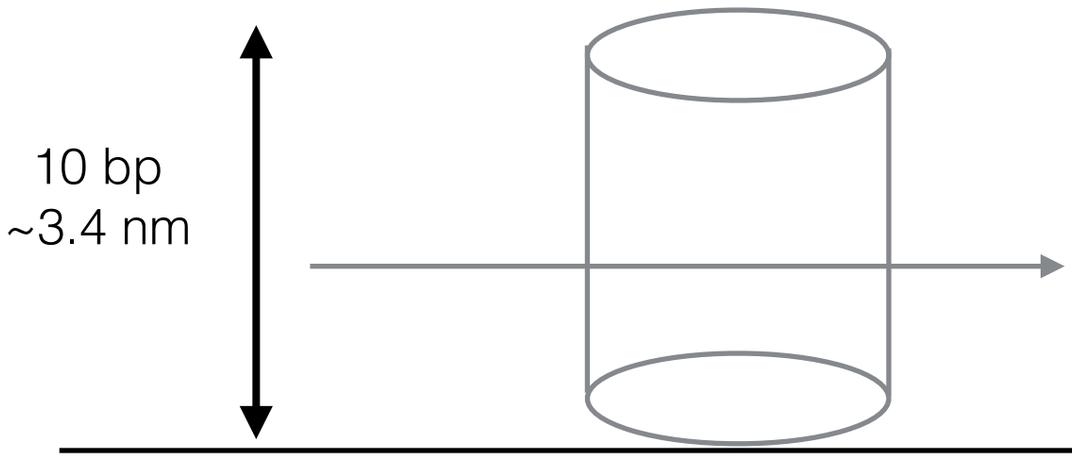

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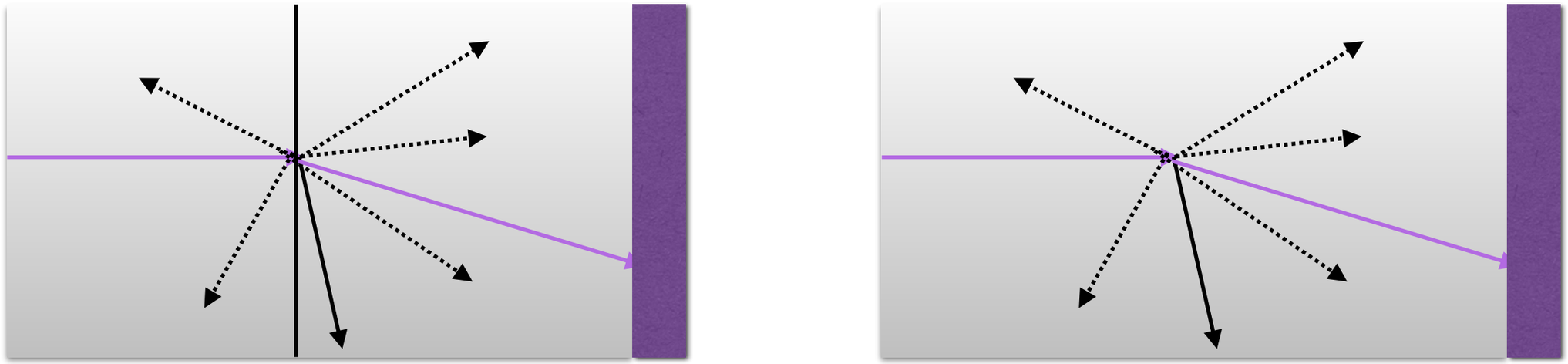

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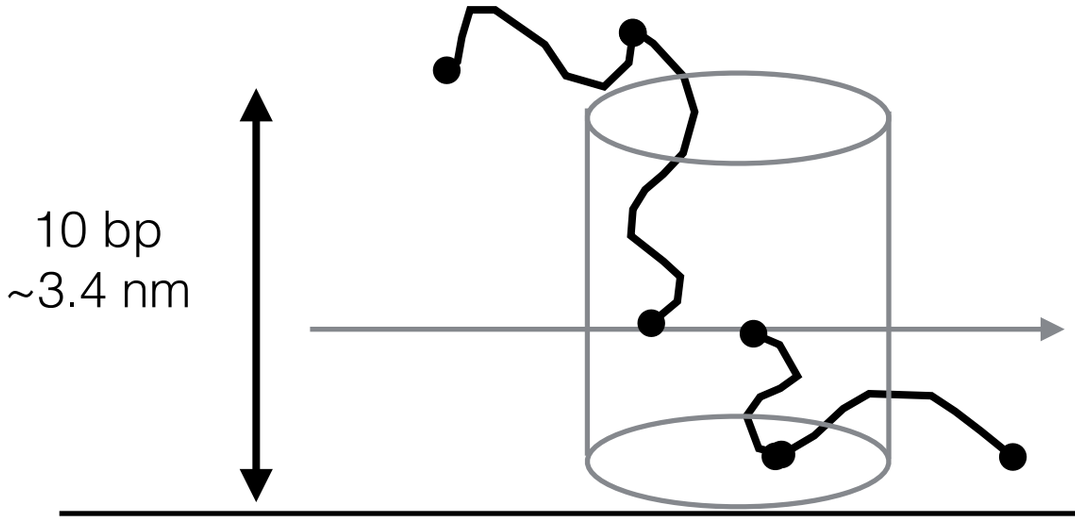

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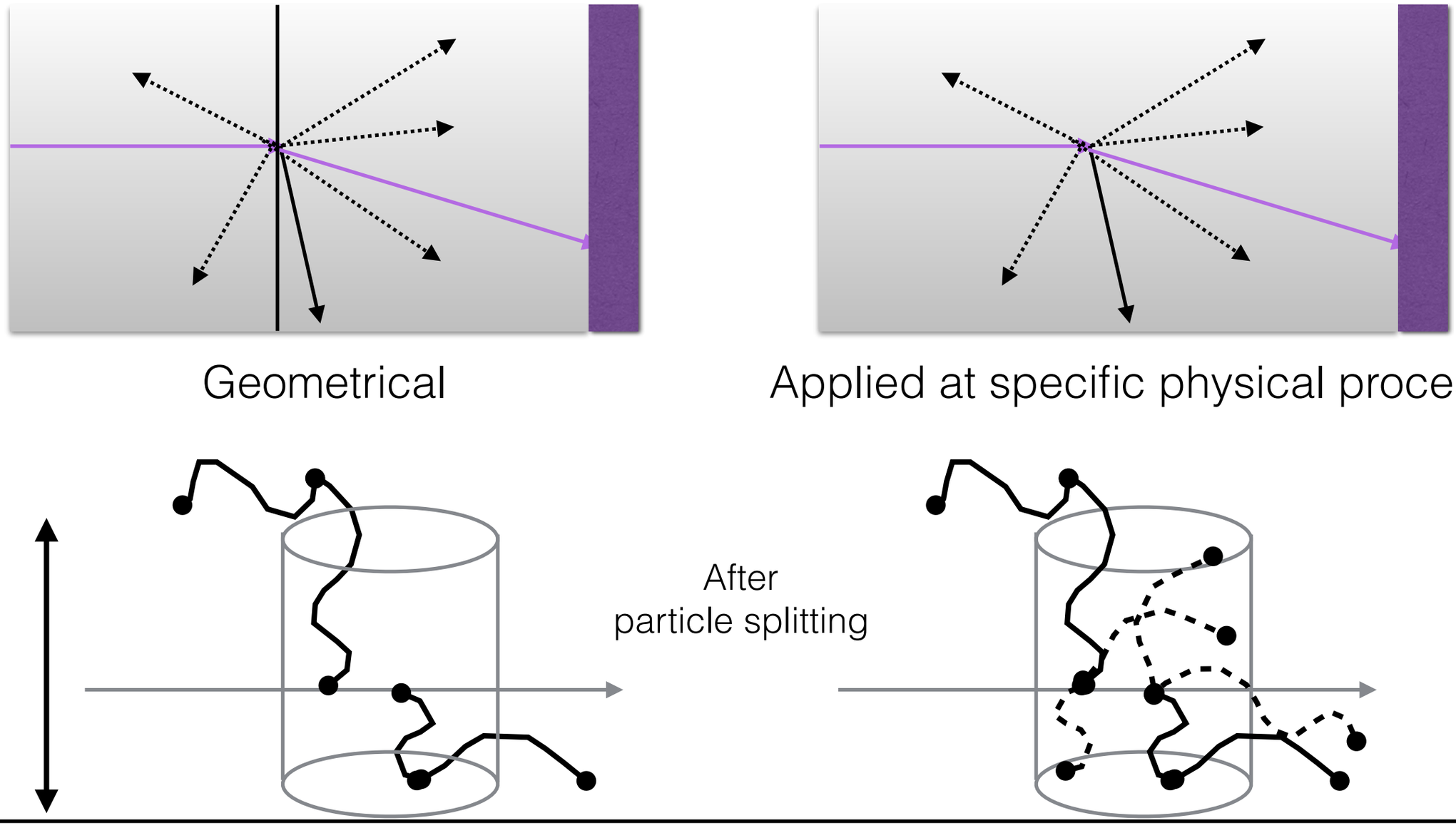

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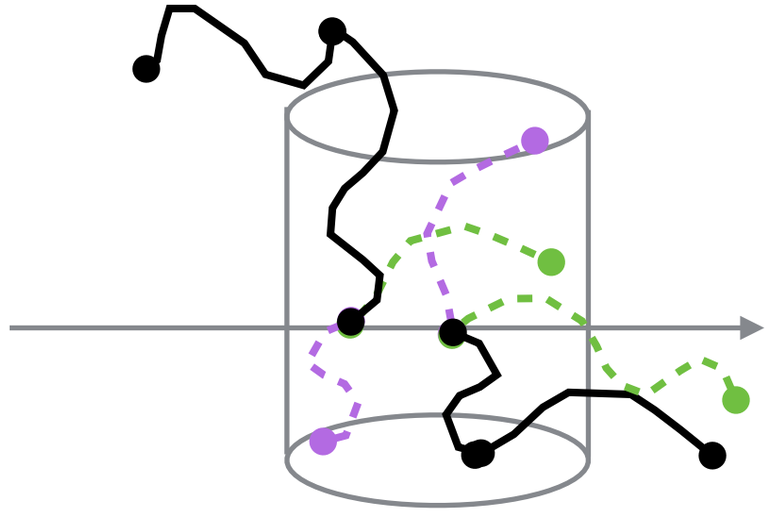
Flagged uniform particle split

- 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



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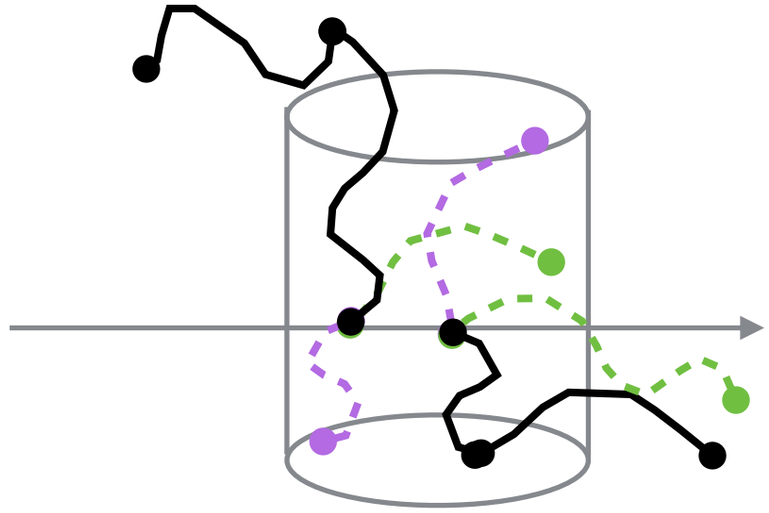
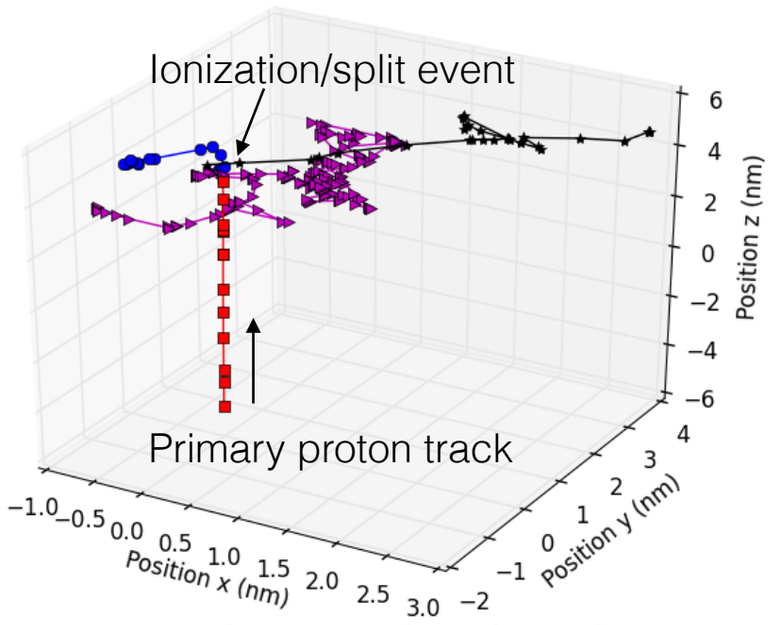


Split N_s=3



primary ionization

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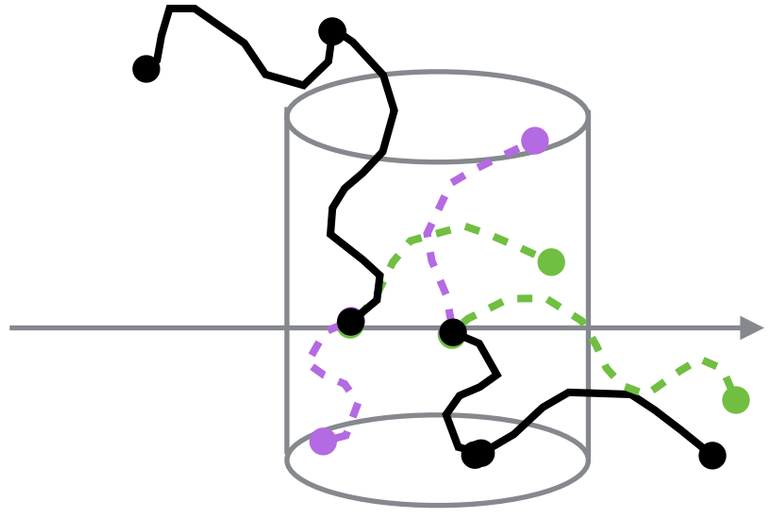

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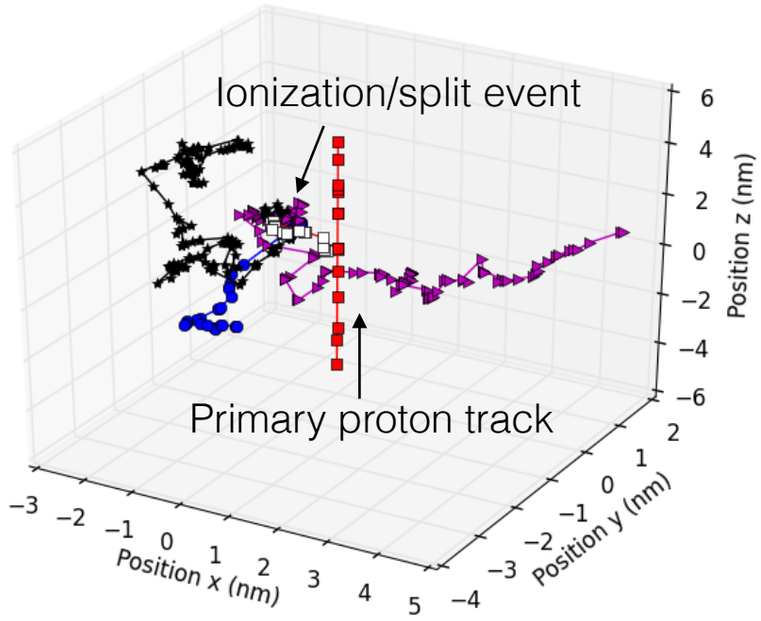
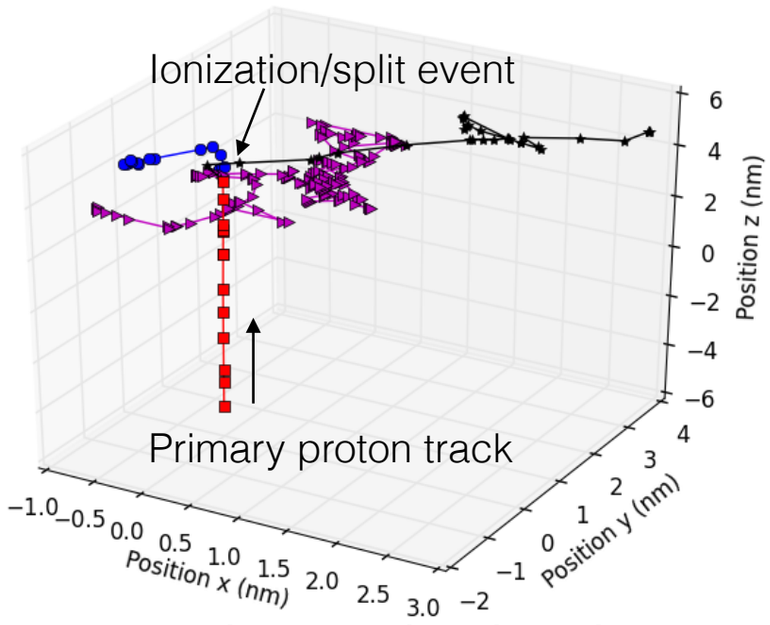


e- ionization



primary ionization

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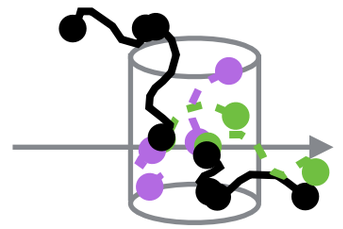
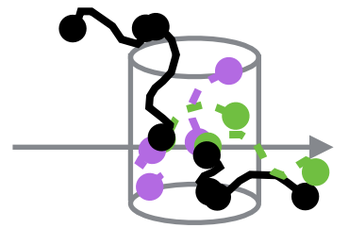


- The split process was implemented by means of the G4WrapperProcess

```
...
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()

Flagged uniform particle split



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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
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 ε of a Monte Carlo simulation, that takes the execution time T to recover the quantity of interest X, with variance σ^2 is given by

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

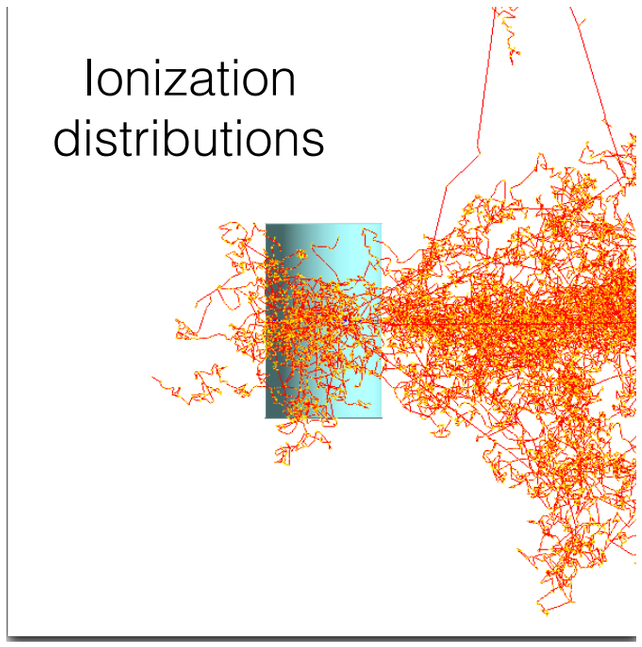
Scoring metric

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 ν is defined as the number of ionizations produced within the scoring region by a single history

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

a) B. Grosswendt and S. Pszona, "The track structure of alpha-particles from the point of view of ionization-cluster formation in 'nanometric' volumes of nitrogen," *Radiat Env. Biophys*, vol. 41, no. 2, pp. 91–102, 2002.

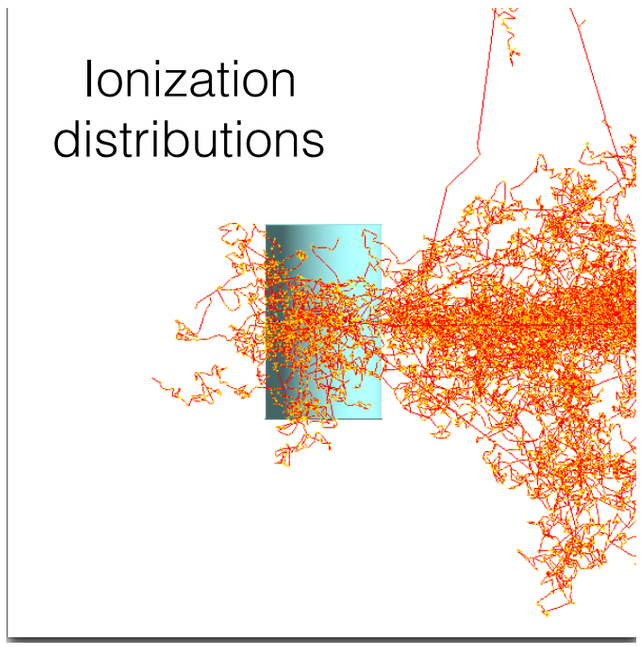
Use cases (Geant4.10.2.p02)



- 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.

a) P. Lazarakis, et. Al "Comparison of nanodosimetric parameters of track structure calculated by the Monte Carlo codes Geant4-DNA and PTra.," *Phys. Med. Biol.*, **57** (5) 1231–50, 2012.

Use cases



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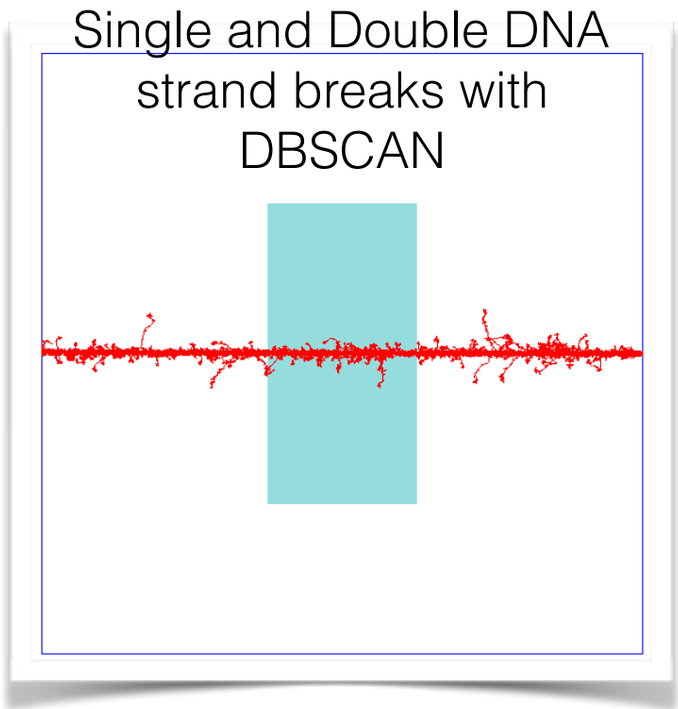
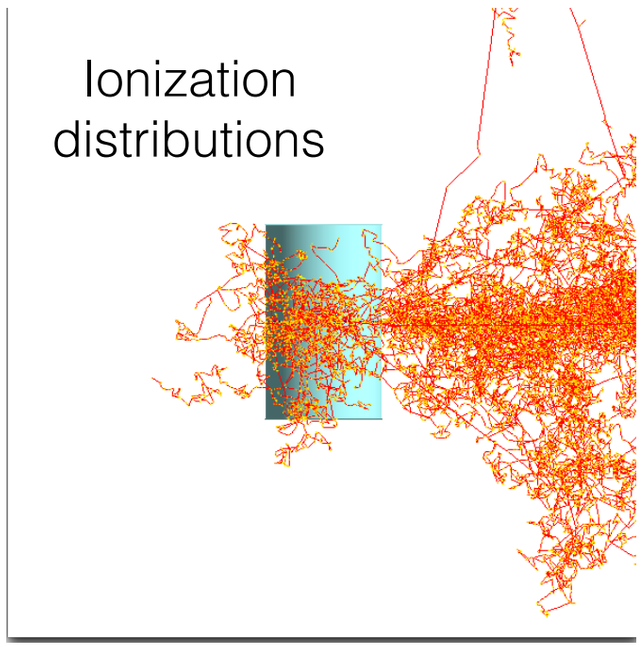


- Box target of 0.5 μm thickness and 1 μm length embedded into a cubic box (World) of 2 μm side.
- DBSCAN parameters: 3.2 nm, E_{min}=5 eV, E_{max}=35 eV, probability of 16% **b)**.
- The number of SSB and DSB per history inside the target was scored.

a) P. Lazarakis, et. Al "Comparison of nanodosimetric parameters of track structure calculated by the Monte Carlo codes Geant4-DNA and PTra.," *Phys. Med. Biol.*, **57** (5) 1231–50, 2012.

b) Z. Francis, et. Al "Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm," *Comput. Methods Programs Biomed.*, **101** (3) 265–270, 2011.

Use cases



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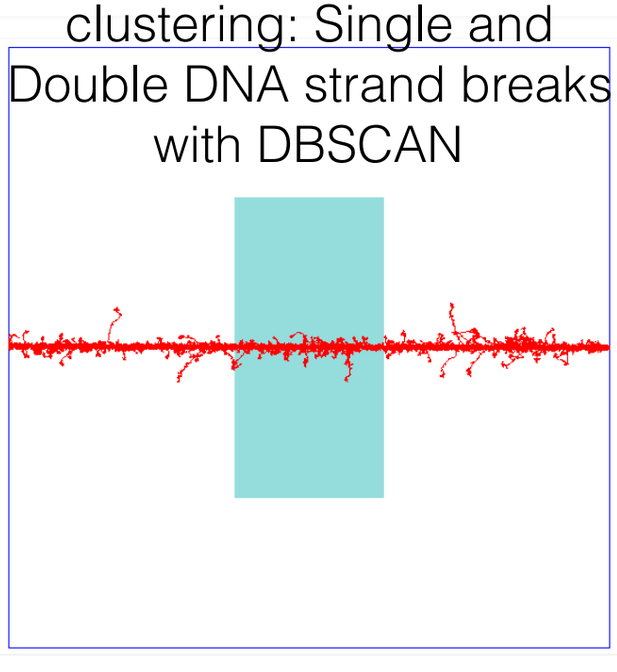
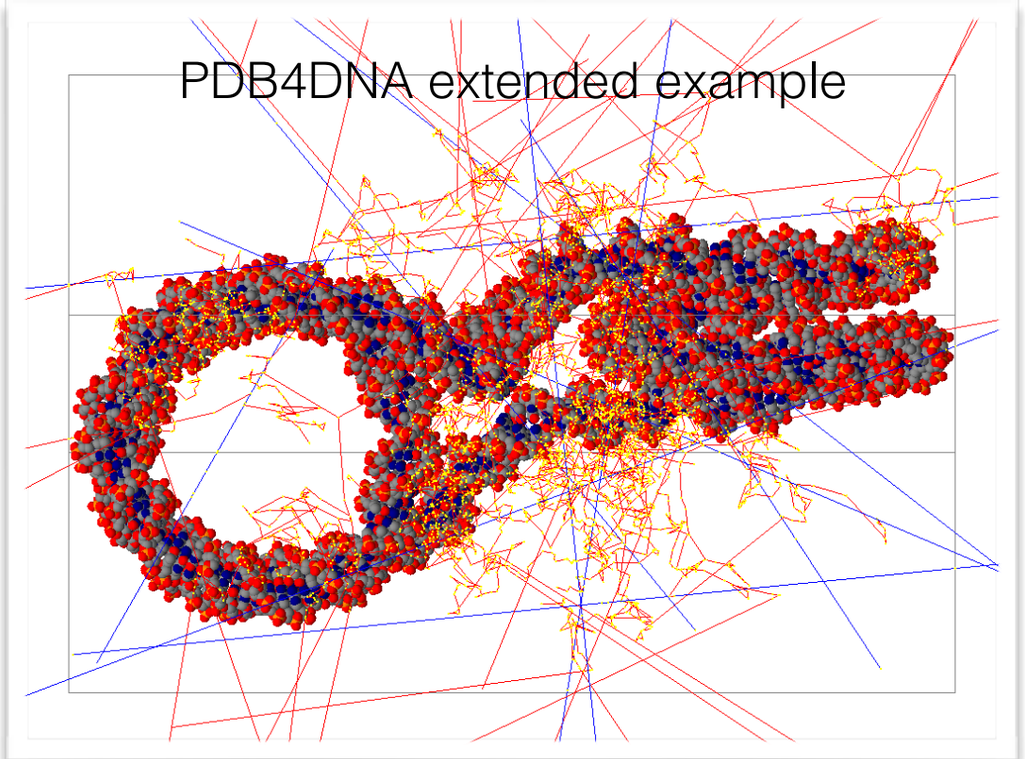


- Box target of 0.5 μm thickness and 1 μm length embedded into a cubic box (World) of 2 μm side.
- DBSCAN parameters: 3.2 nm, E_{min}=5 eV, E_{max}=35 eV, probability of 16% **b)**.
- The number of SSB and DSB per history inside the target was scored.



- Box target of 9.71 x 7.61 x 12.63 nm3 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

a) P. Lazarakis, et. Al "Comparison of nanodosimetric parameters of track structure calculated by the Monte Carlo codes Geant4-DNA and PTra.," *Phys. Med. Biol.*, **57** (5) 1231–50, 2012.

b) Z. Francis, et. Al "Simulation of DNA damage clustering after proton irradiation using an adapted DBSCAN algorithm," *Comput. Methods Programs Biomed.*, **101** (3) 265–270, 2011.

c) E. Delage, et. Al "PDB4DNA: Implementation of DNA geometry from the Protein Data Bank (PDB) description for Geant4-DNA Monte-Carlo simulations," *Comput. Phys. Commun.*, **192**, 282–288, 2015.

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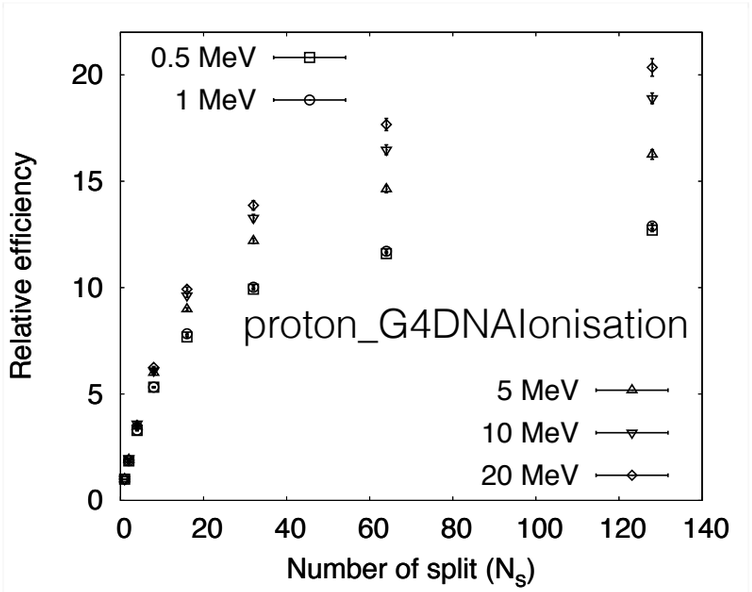
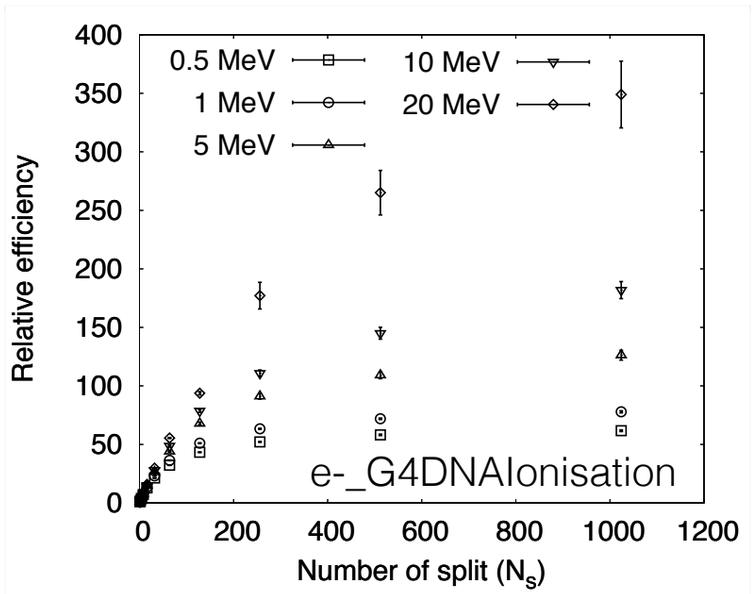
Results: protons

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.





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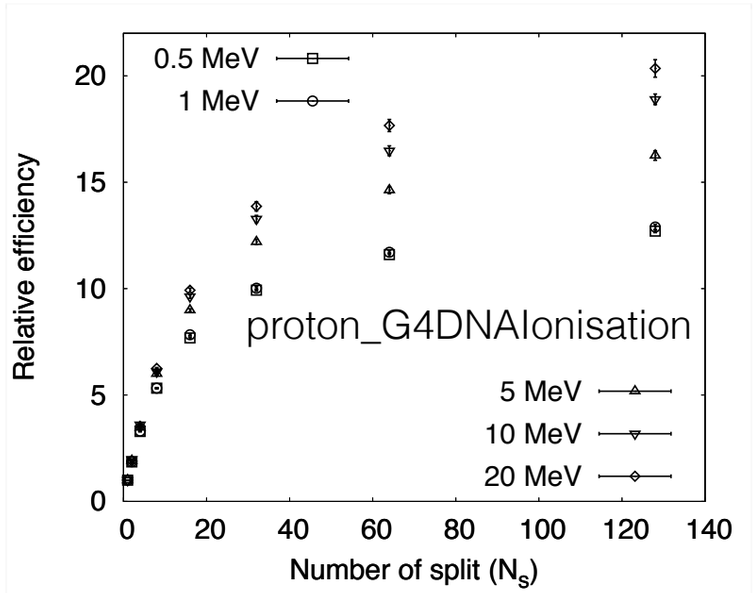
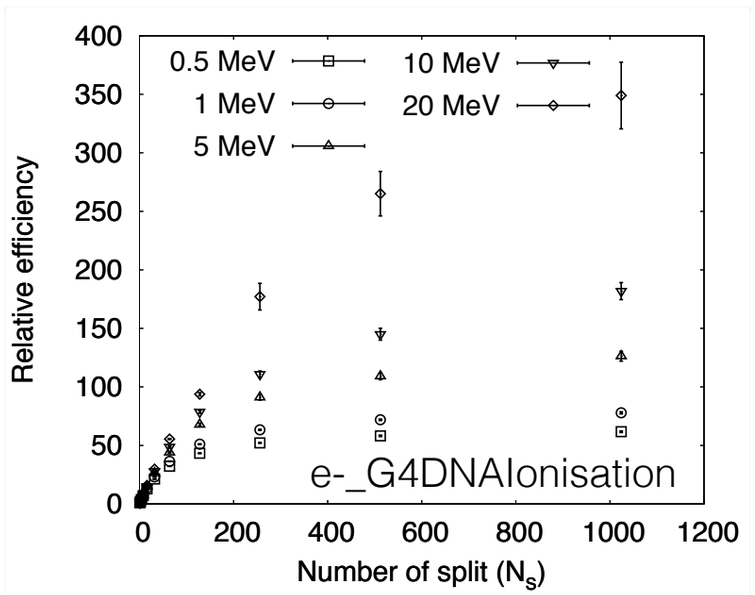
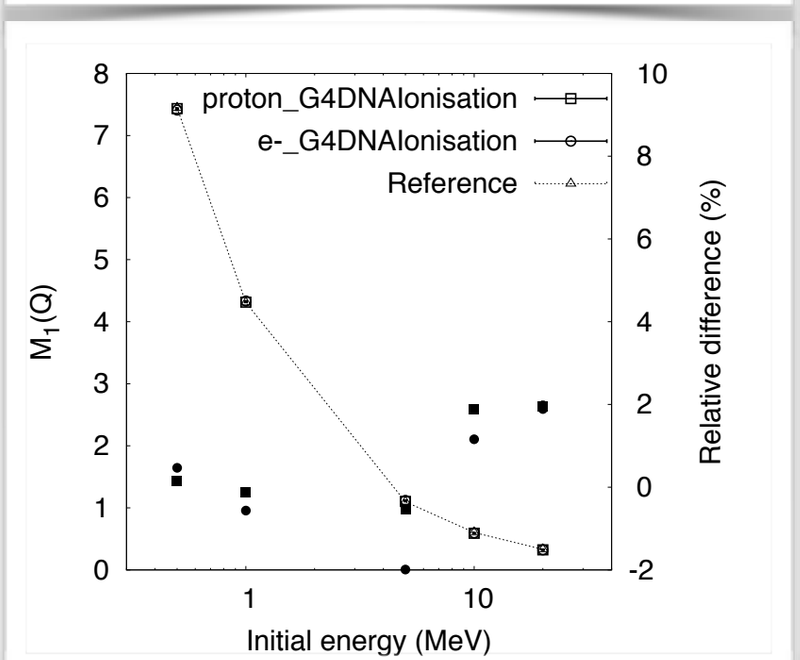
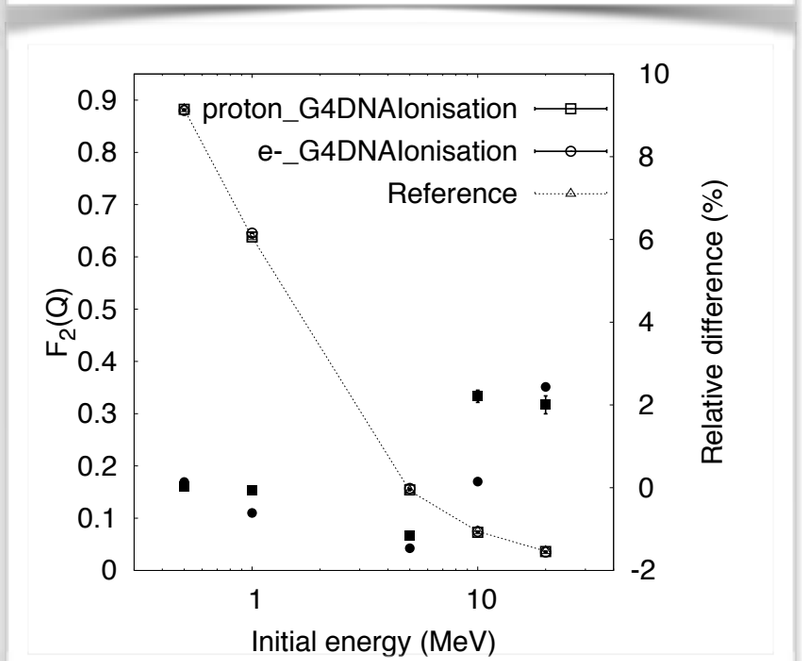


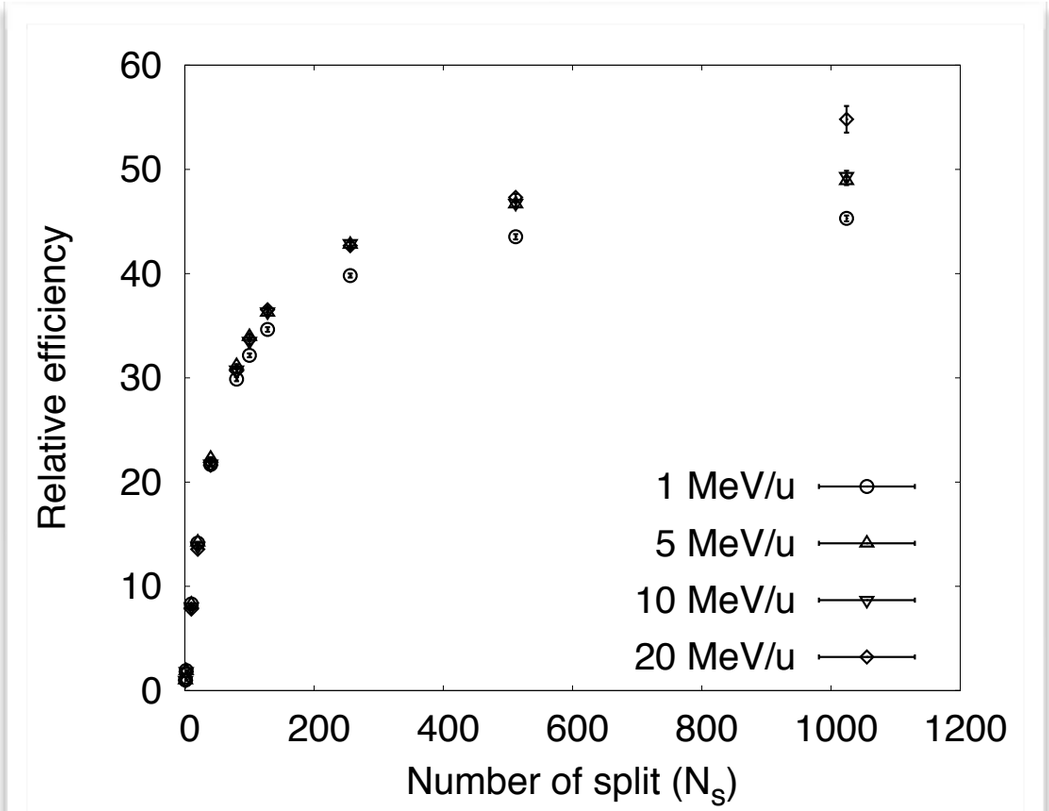




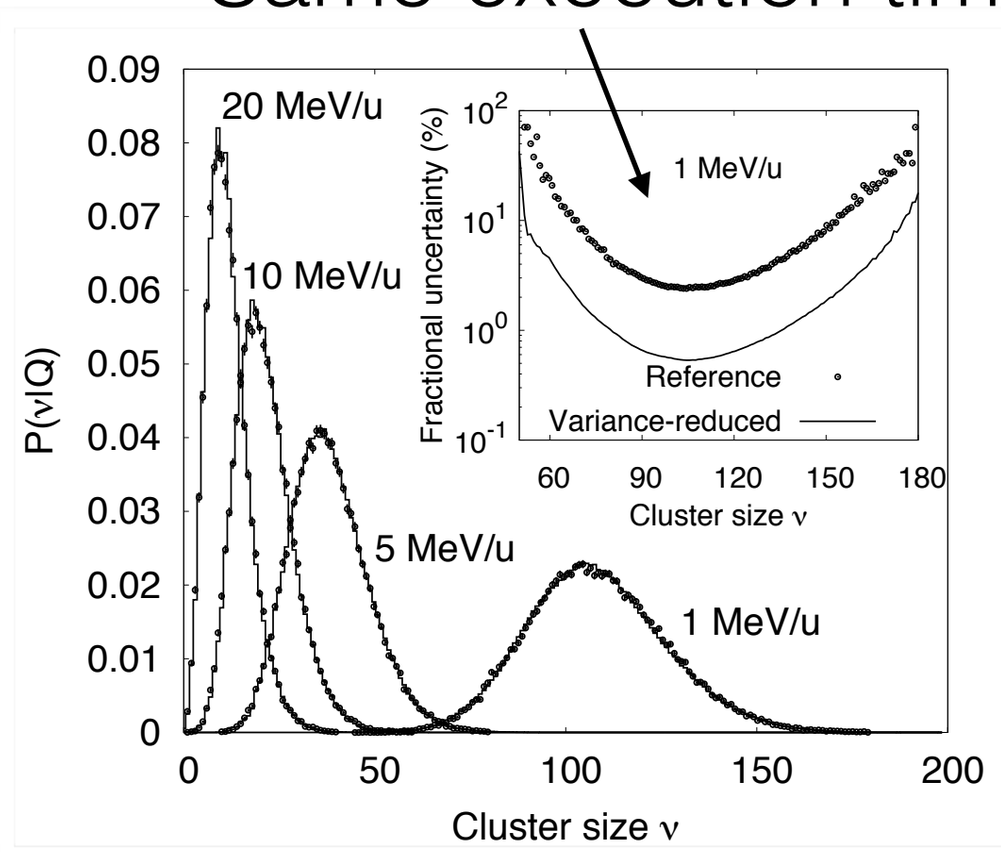


Bottom: First moment $M_1(Q)$ and cumulative distribution $F_2(Q)$ of $P(\nu|Q)$ in function of the kinetic energy of the proton for the two physical process improved with the flagged uniform particle split. In both cases, on the right axis is shown the relative difference (filled markers) with respect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

Results: Carbon ions



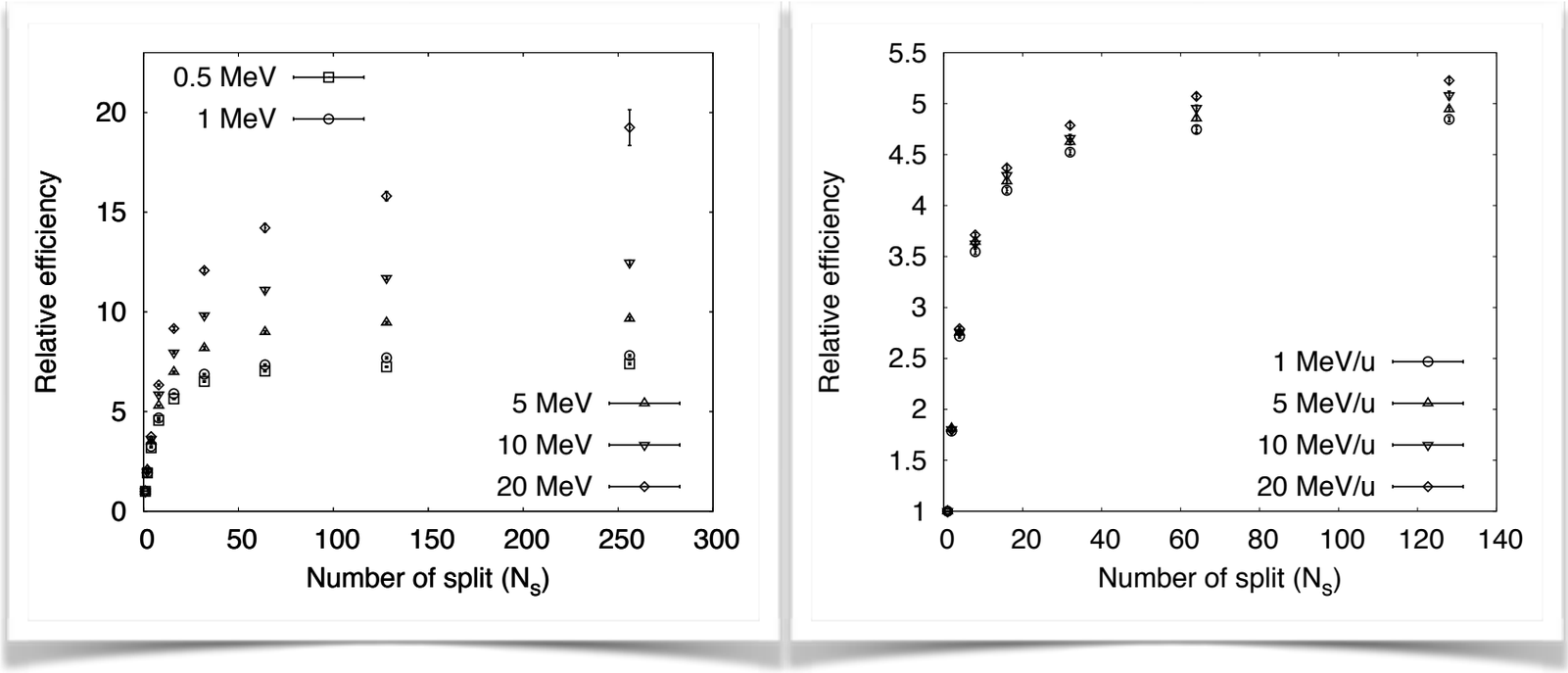
Same execution time



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 **`e-_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.

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.



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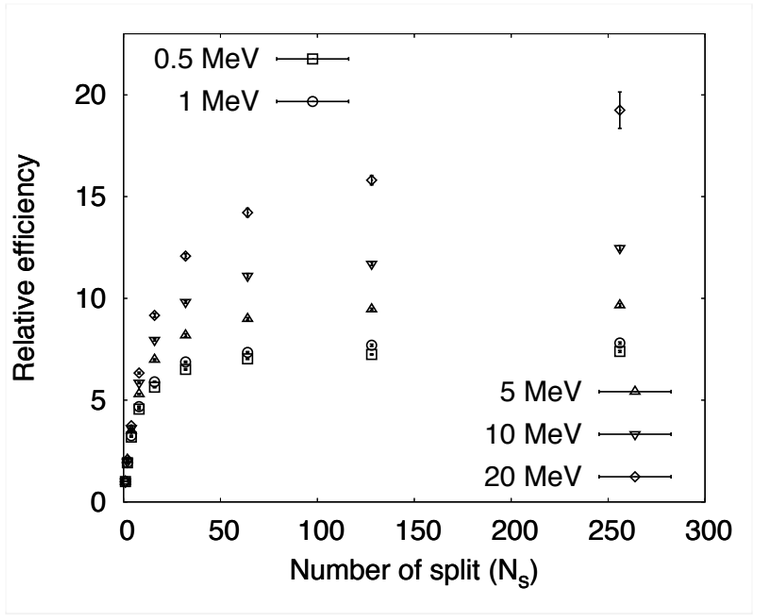
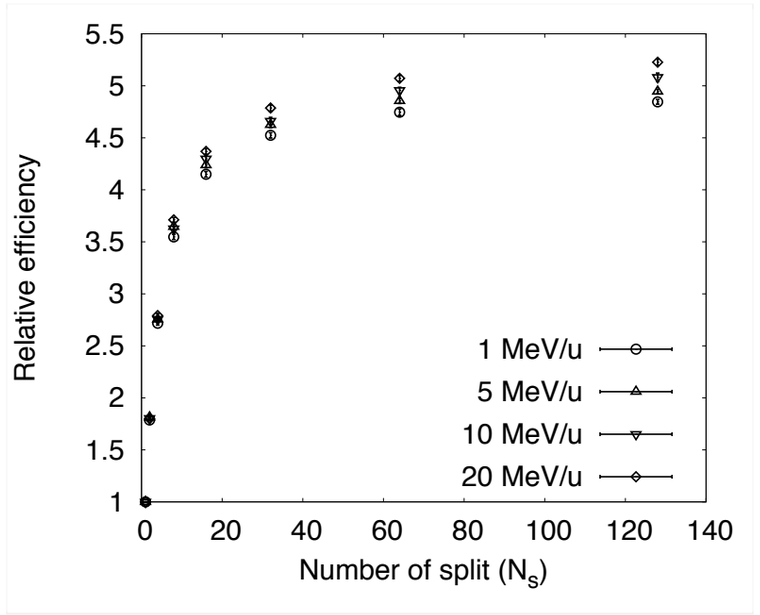
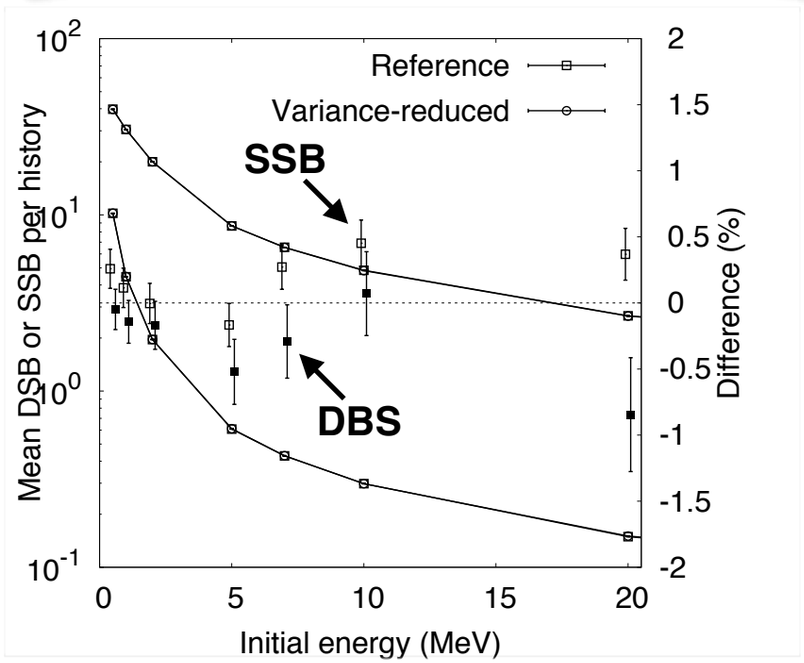
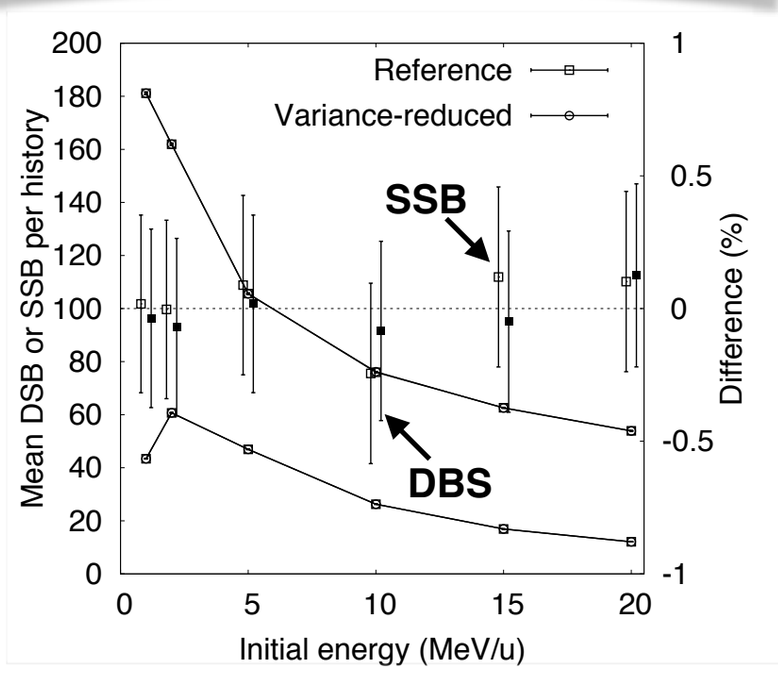




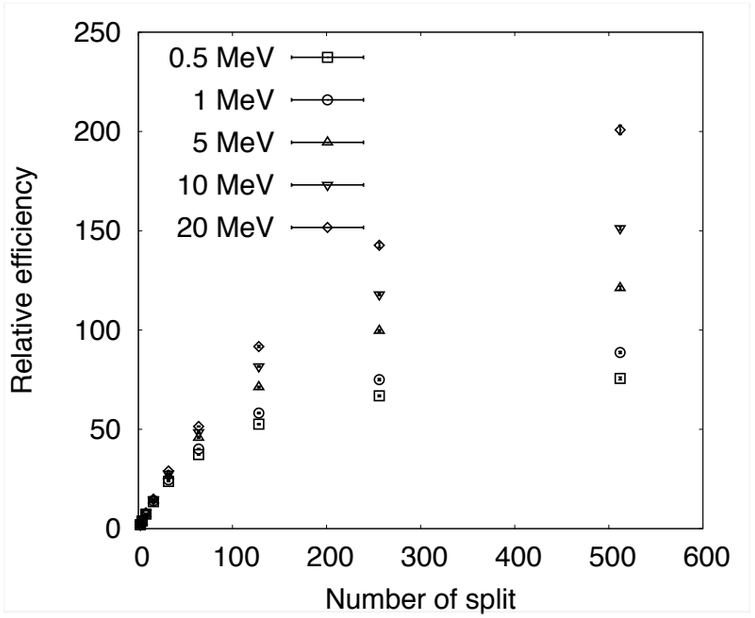


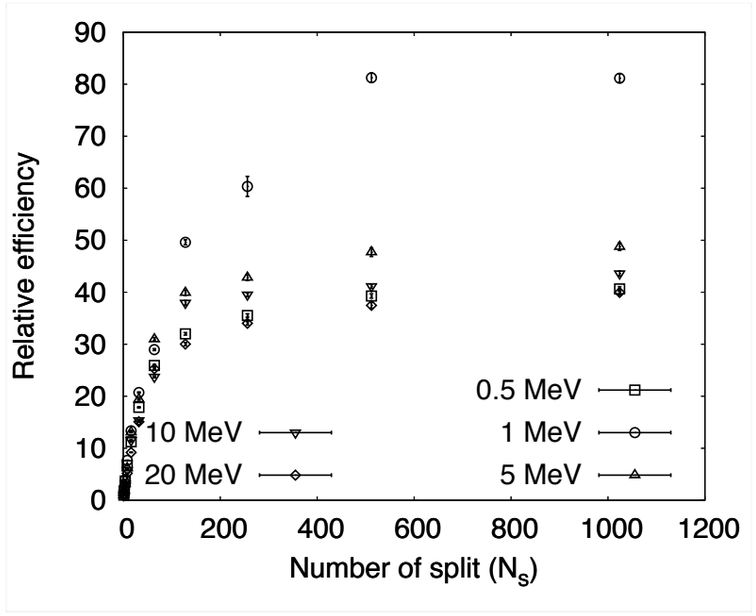


Bottom: The mean number of DBS and SSB for proton energies from 0.5 to 50 MeV and carbon ions from 1 to 20 MeV/u are shown. Lines are for guide the eyes. The flagged uniform particle split was applied with N_s=64 for protons and N_s=32 for carbon ions. The relative difference in percent is shown on the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

Results: PDB4DNA

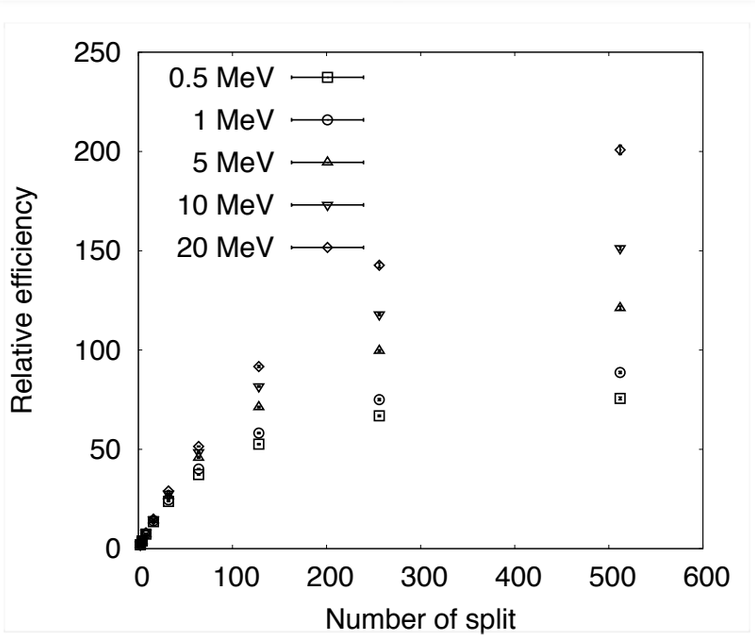
Top: Relative efficiency versus the number of split N_s for several energies of the incoming proton (left) and carbon ion (right) source.The error bars represent one standard deviation.

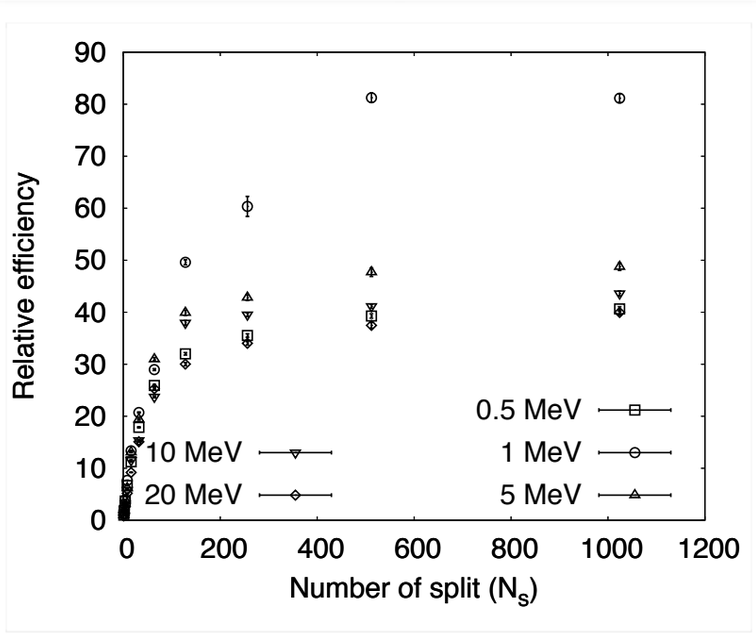


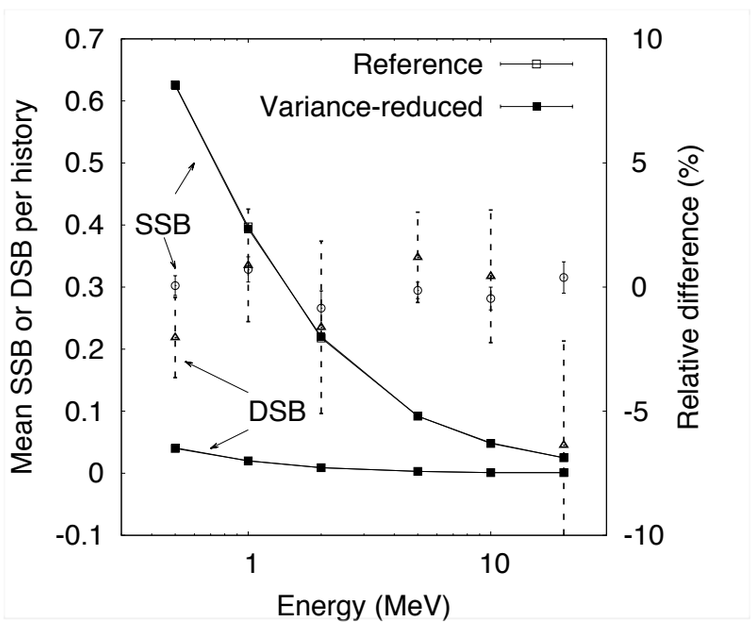


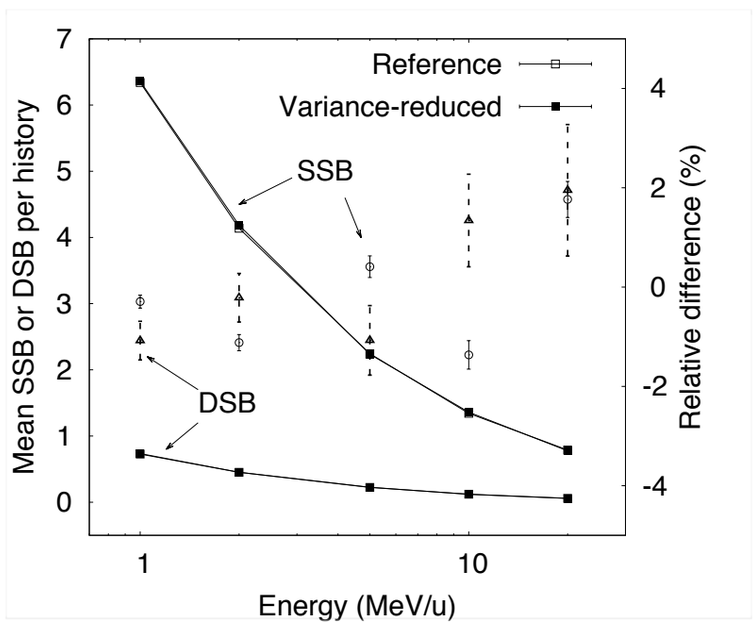
Results: PDB4DNA

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

UCSF Medical Center

UCSF Benioff Children's Hospitals

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.