

V. Maulerova-Subert, I. Dawson, E. Garutti, M.Moll, A. Himmerlich, Y. Gurimskaya

NIEL(non-ionizing energy loss)

Geant4 simulations and OPTICS algorithm towards more complex NIEL concept for radiation damage modelling and prediction





The 40th RD-50 workshop, CERN, 21.06.2022

CONTENTS

- 1. The NIEL hypothesis: concept explanation and its shortcomings.
- 2. **Geant4** simulation framework
- 3. Primary knocked-on atoms (PKA)
- 4. OPTICS (Ordering points to identify the clustering structure) algorithm
- 5. Secondary knocked-on atoms (SKA)
- 6. Summary and next steps

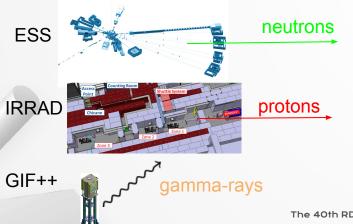
The NIEL hypothesis

The 40th RD-50 workshop, CERN, 21.06.2022

à à à à

NIEL (non-ionizing energy loss)

- NIEL is a physical quantity describing the non-ionizing energy loss as the particle travels through the medium.
- The amount of NIEL can be correlated to the ammount of radiation damage (NIEL scaling model) and therefore to predict the life time of the detectors.
- **NIEL** is usually expressed as an equivalent to **NIEL** of 1 MeV neutrons.



• NIEL scaling assumption is used by most of the LHC experiments

Long term goal: to revisit the damage factor stated by different irradiation facilities

NIEL (non-ionizing energy loss)

Displacement damage function

$$NIEL(T_0) = rac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T) Tig(rac{d\sigma}{dT}ig)_i dT$$

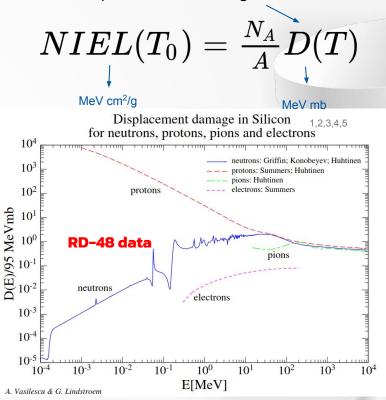
- **T**₀: energy of incident particle
- **T**: energy transferred to the recoil atom
- (dσ/dT): differential partial cross section for a particle with energy T₀ to create a recoil atom with energy T in the i-th reaction
- **Q(T)**: partition factor giving the fraction of **T** that is going into further displacements
- N_A : Avogadro number

1)

4)

• A : atomic mass of target atom

 Summers, G. P., E. A. Burke, P. Shapiro, et al. "Damage Correlations in Semiconductors Exposed to Gamma, Electron and Proton Radiations." IEEE Transactions on Nuclear Science, vol. 40, no. 6, Dec. 1993, pp. 1372–79. IEEE Xplore, https://doi.org/10.1109/23.273529.



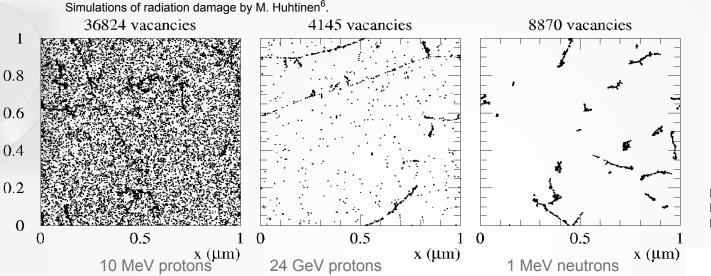
Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg)

²⁾ P.J. Griffin et al., SAND92-0094 (Sandia Natl. Lab.93), priv. comm. 1996: E = 1.025E-10 - 1.995E+01 MeV

³⁾ Konobeyev, Alexander Yu., et al. "Nuclear Data to Study Damage in Materials under Irradiation by Nucleons with Energies up to 25 GeV." Journal of Nuclear Science and Technology, vol. 39, no. sup2, Aug. 2002, pp. 1236–39. Taylor and Francis+NEJM, https://doi.org/10.1080/00223131.2002.10875327.

Huhtinen, M., and P. A. Aarnio. "Pion Induced Displacement Damage in Silicon Devices." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 335, no. 3, Nov. 1993, pp. 580–82.
ScienceDirect, https://doi.org/10.1016/0168-9002(93)91246-J.

Revisiting NIEL



Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons⁷.

EPI p-type Si, 250 Ω·cm, 10min@60°C, V_{biac}=-100V

100

Temperature (K)

signal (pA) 50

LSC:

10

- protops 7 80E+11

V in cluster

• NIEL doesn't distinguish between cluster and point displacement, i.e. the same displacament energy has a very different distribution of damage on the microscopic level.

y (µm)

• NIEL scaling violation reported in oxygen enriched silicon samples (CERN RD-48), differences between neutron's and proton's damage

6) Huhtinen, M. "Simulation of Non-Ionising Energy Loss and Defect Formation in Silicon." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 491, no. 1, Sept. 2002, pp. 194–215. ScienceDirect, https://doi.org/10.1016/S0168-9002(02)01227-5.

7) Gurimskaya, Yana, et al. "Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 958, Apr. 2020, p. 162221. ScienceDirect, https://doi.org/10.1016/j.nima.2019.05.062.

Geant4 simulations

The 40th RD-50 workshop, CERN, 21.06.2022

Geant4 simulation framework

Geant4^{8,9}(for GEometry ANd Tracking) is a Monte Carlo simulation platform for the passage of particles through matter.

Define a geometry:

For most of the simulations: 1mm x1 mm x100 µm

Define a beam profile:

Choose a physics list:

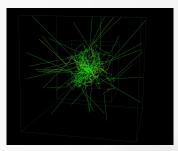
1. For PKA:

- a. *QGSP_BERT_HP* (Nuclear scattering)
- b. *QGSP_BERT_HP__SS* (Coulomb scattering)
- 2. For subsequent cascade:
 - a. Custom PhysicsList¹⁰
- 1. For PKA: Monochromatic pencil beam of protons and neutrons of various energies.
- 2. For subsequent cascade: Single Si particles of various energies being injected

Analyze (c++, python)

Launch a simulation:

QGSP_BERT_HP QGSP_BERT_HP__SS Custom Physics¹⁰



8) Agostinelli, S., et al. "Geant4—a Simulation Toolkit." Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, D Detectors and Associated Equipment, vol. 506, no. 3, July 2003, pp. 250–303. ScienceDirect, https://doi.org/10.1016/S0168-9002(03)01368-8.

9) Allison, J., K. Amako, J. Apostolakis, H. Araujo, et al. "Geant4 Developments and Applications." IEEE Transactions on Nuclear Science, vol. 53, no. 1, Feb. 2006, pp. 270–78. IEEE Xplore, https://doi.org/10.1109/TNS.2006.869826.

10) Raine, Melanie, et al. "Simulation of Single Particle Displacement Damage in Silicon - Part I: Global Approach and Primary Interaction Simulation." IEEE Transactions on Nuclear Science, vol. 64, no. 1, Oct. 2016, pp. 133–40. HAL Archives Ouvertes, https://doi.org/10.1109/TNS.2016.2615133.

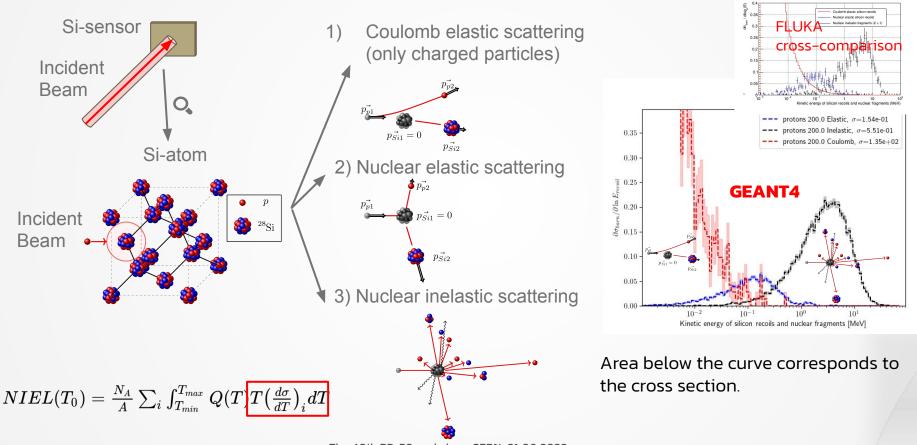
PKA (Primary knocked-on atoms)

The 40th RD-50 workshop, CERN, 21.06.2022

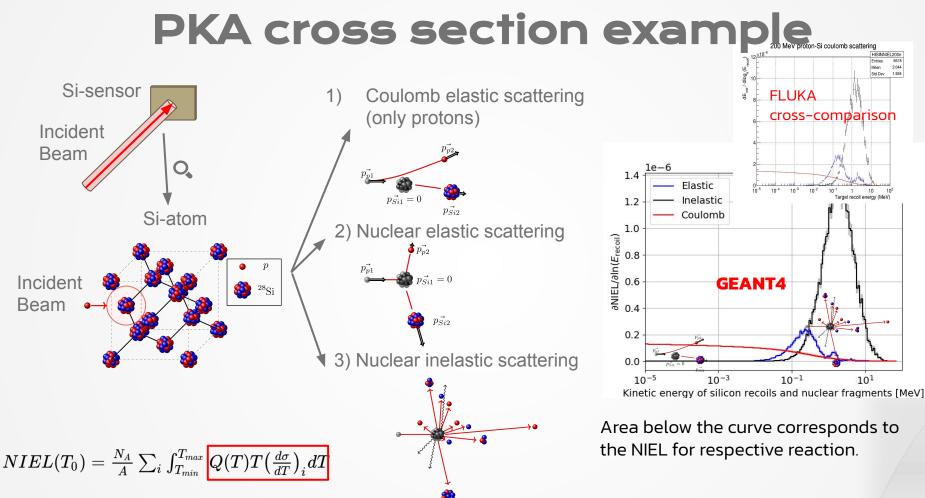


۲ 🙆

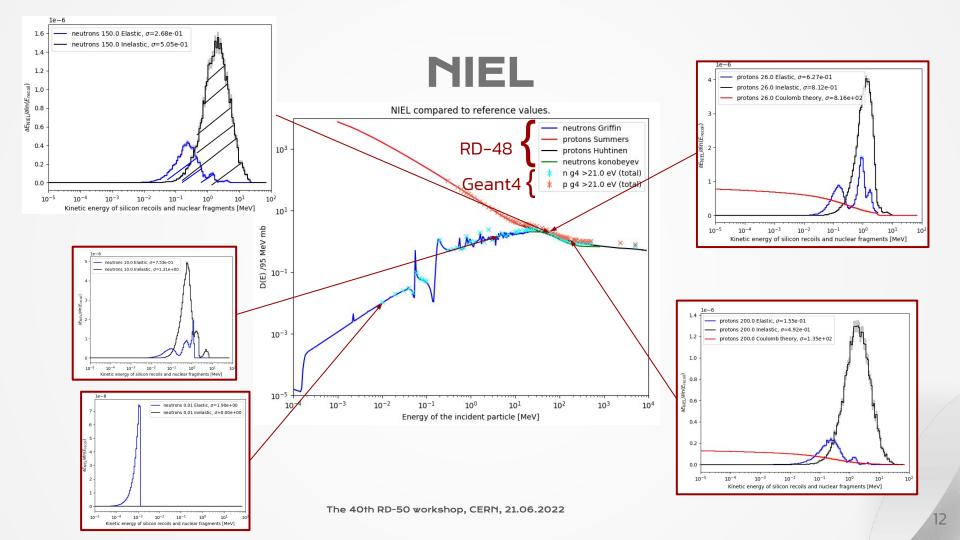
PKA cross section example

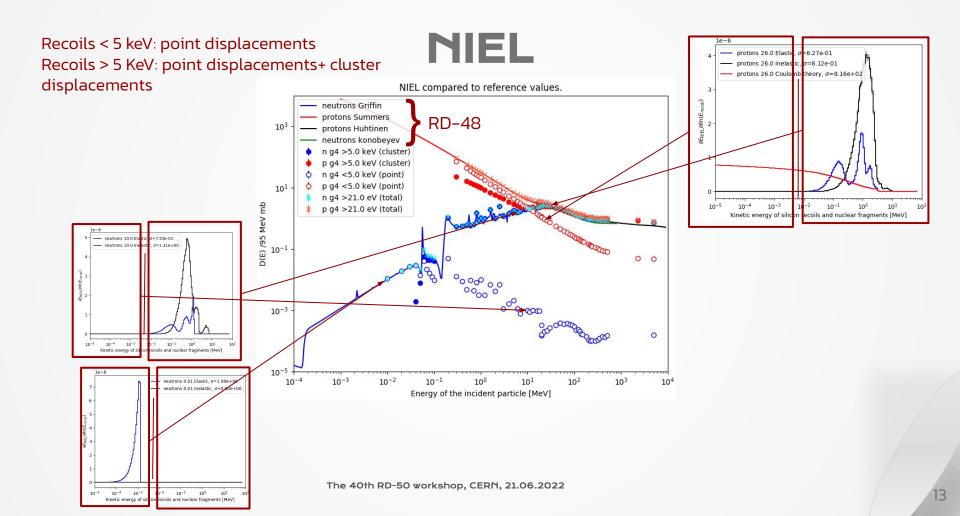


200 MeV Protons



The 40th RD-50 workshop, CERN, 21.06.2022





SKA Secondary knocked-on atoms)

The 40th RD-50 workshop, CERN, 21.06.2022

🥸 🥸

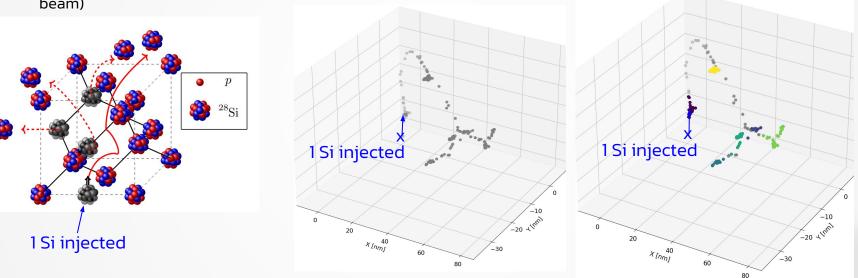
How to define a cluster? What algorithm to choose?

- Geant4 studies with Screened Nuclear Recoil process¹⁰
- focus on the propagation of Si-recoil in Silicon (no incident beam)

Example:

- 100 keV Silicon track
- originating from the blue cross (position 0,0,0)
- initial momentum in +z direction

Grey dots: isolated displacements Colored dots: clustered displacements



10) Raine, Melanie, et al. "Simulation of Single Particle Displacement Damage in Silicon - Part I: Global Approach and Primary Interaction Simulation." IEEE Transactions on Nuclear Science, vol. 64, no. 1, Oct. 2016, pp. 133–40. HAL Archives Ouvertes, https://doi.org/10.1109/TNS.2016.2615133.

Clusters

- Cluster detection is a big topic in machine learning and mathematics
- Depending on its application, different algorithms are the best fit.

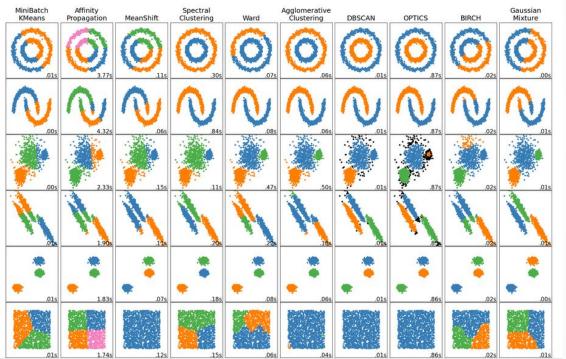


Image from^{11,12}

- Various clustering algorithms applied to 6 different sample datasets
- aim : identify clusters
- Algorithm must be able to process:
 - samples with large number of "outliers" (=single displacements for us)
 - samples with clusters of different shapes
 - samples with clusters with various densities

11) Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. *Journal of Machine Learning Research*, *12*, 2825–2830.

 $\label{eq:linear} 12) https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison n.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py$

The 40th RD-50 workshop, CERN, 21.06.2022

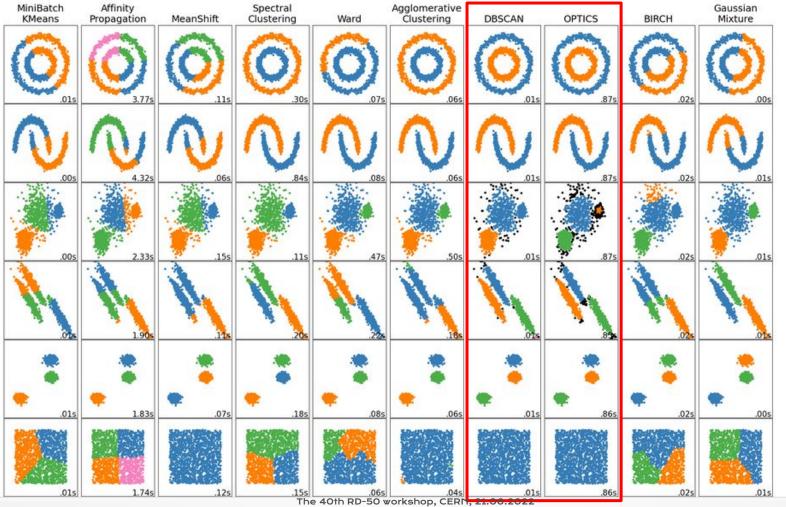


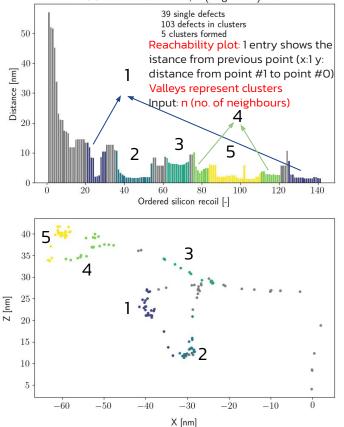
Image from^{11,12}

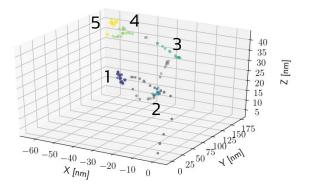
OPTICS performs better then DBSCAN for clusters with varying densities¹³.

11) Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... Duchesnay, E. (2011). Scikit-learn: Machine Learning in Python. Journal of Machine Learning Research, 12, 2825-2830. 12)https://scikit-learn.org/stabl

e/auto examples/cluster/plot cluster comparison.html#sph x-glr-auto-examples-cluster-pl ot-cluster-comparison-py 13)https://scikit-learn.org/stabl e/modules/clustering.html#opt ics

OPTICS^{13,14} (Ordering points to identify the clustering NO keV incident recoil, n (neighbours)= 9 structure)





- Algorithm flow explain in the Appendix (Slide 31)
- Basic idea:
 - Ordering points and plotting their distances produces **Reachability plot**
 - Valleys in the reachability plot represent clusters
- Algorithm needs a user input: minimum number of samples to create cluster

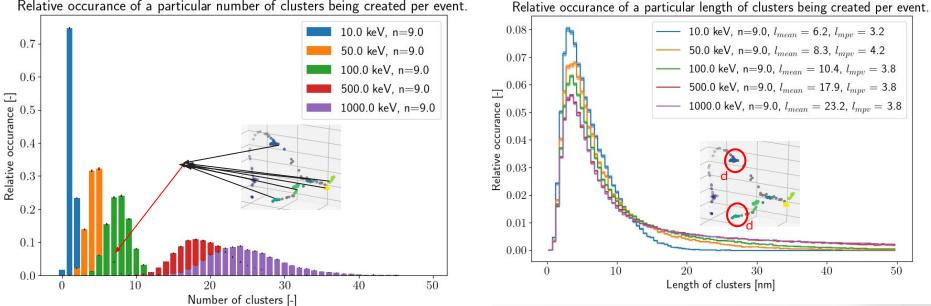
Ankerst, Mihael, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. "OPTICS: ordering points to identify the clustering structure." ACM SIGMOD Record 28, no. 2 (1999): 49-60.
Schubert, Erich, Michael Gertz. "Improving the Cluster Structure Extracted from OPTICS Plots." Proc. of the Conference "Lernen, Wissen, Daten, Analysen" (LWDA) (2018): 318-329.
<u>https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s</u> tutorial

RESULTS

How many clusters?

How large are the clusters?

Length := diameter of the smallest enclosed sphere around the cluster



Relative occurance of a particular number of clusters being created per event.

- If the cluster is too big, the algorithm prefers to break the cluster down into a smaller subclusters. •
- While the cluster size remains similar with energy, the number of clusters increases.

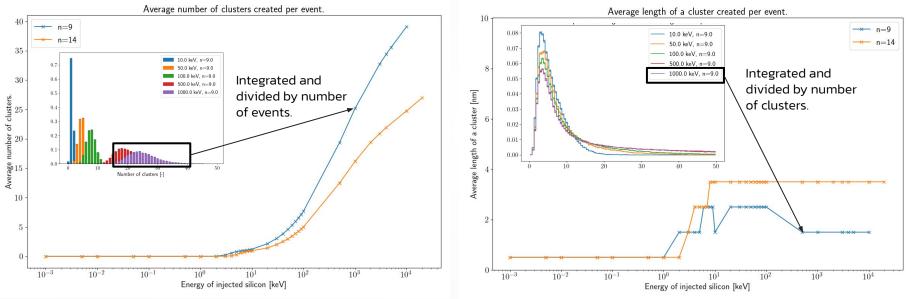
RESULTS

How many clusters?

How large are the clusters?

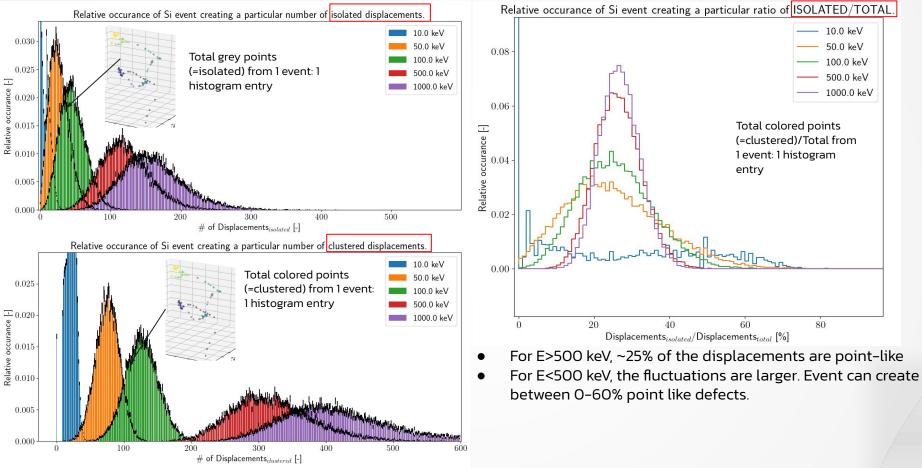
Length := diameter of the smallest enclosed sphere around





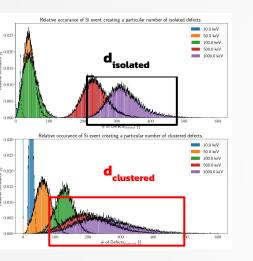
- For Si > 10 keV the length of the cluster for $n=14 \sim 3 \text{ nm}$, for Si > 10 keV the length of the cluster for $n=9 \sim 1-2 \text{ nm}$.
- For n=9 the algorithm detects higher number of clusters with smaller sizes, for n=14 it is the opposite.

RESULTS



The 40th RD-50 workshop, CERN, 21.06.2022

By integrating plots from previous slide for respective energies and dividing by the number of histogram entried, we gain 1 point on the plot on the right plot.



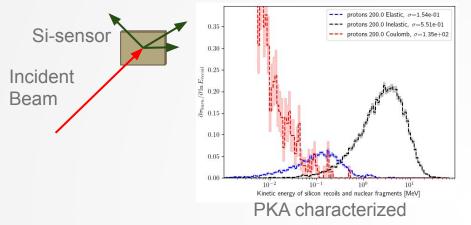
- For E > 50 keV stable ratio of point-like and cluster displacements are independent of the choice of n
- The threshold energy for creating stable ratio of point-like and cluster displacements depends on the algorithm parameter.

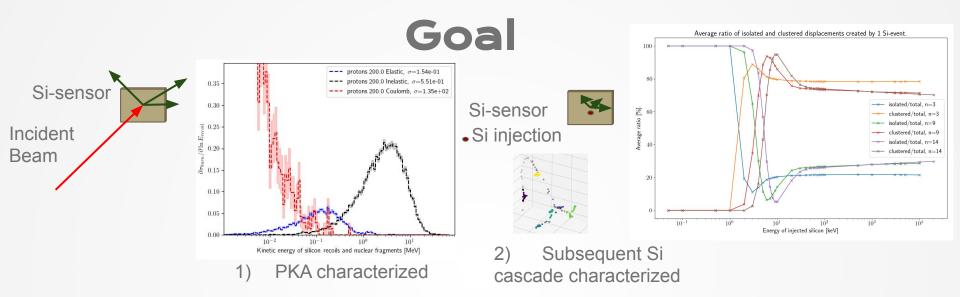
RESULTS

Average ratio of isolated and clustered displacements created per event. 100 Total number of d_{clustered}/(d_{isolated}+d_{clustered}) 80 isolated/total, n=360 clustered/total, n=3isolated/total, n=9 clustered/total, n=9 Total number of isolated/total, n=14 ~ - - - 40 d isolated / (d isolated + d clustered \leftarrow clustered/total, n=14 20 0 10^{0} 10^{-1} 10^{2} 10^{3} 10^{4} 10^{1} Energy of injected silicon [keV]

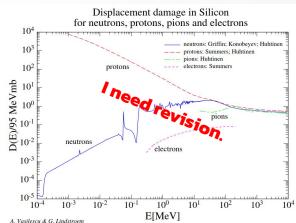
Average ratio [%].

Goal

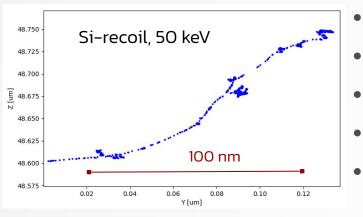




- 3) Goal:
 - take the output of 1) for all projectile energies and apply the output of 2) subsequent Si cascade.
 - A revised version of RD48 should show the cluster vs isolated defect contribution.
 - At this point benchmark with measurements will be possible.



Outlook & next steps



- A Geant4-based simulations and analysis are being carried out together with FLUKA to revisit the RD-48 NIEL curves.
- NIEL curves in literature with Geant4 and Fluka simulations successfully reproduced
- Algorithm for identifying clustered versus point defect damage implemented.
- For Si recoil of the energy above 50 keV energy threshold the cluster to point defect ration remains constant, in agreement with the literature¹⁴.
- Further developments of algorithm for damage differences between different particles are envisioned.
 - Closure on cluster's parameter definition.
 - Further studies and comparisons with FLUKA.
 - Cluster/Isolated displacements containing update of the RD48 plot for protons and neutrons and extending studies to electrons and gammas.
- Benchmarking with DLTS measurements data.
- Determine fraction of cluster NIEL in irradiation facilities, e.g. CERN PS versus JSI research reactor.

THANKS!

Do you have any questions?

The 40th RD-50 workshop, CERN, 21.06.2022

Extra slides

87

Geant4 physics list, step functions

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi Ecole Polytechnique - LLR

For physics list:

- AtRest functions: decay, e+ annihilation
- AlongStep functions: to describe continuous (inter)actions, occurring along the path of the particle, like ionisation
- PostStep actions: For describing point-like (inter)actions, like decay in flight, hard Radiation..

G4VProcess: can implement any combination of AtRest, AlongStep, PostStep action

GetPhysicalInteractionLength():

- Used to limit the step size:
- either because the process « triggers » an interaction, a decay;
- Or any other reasons, like fraction of energy loss;
- geometry boundary;
- user's limit ..

8) https://geant4.web.cern.ch/sites/default/files/geant4/collaboration/workshops/users2002/talks/lectures/PhysicsProcessesInGeneral.pdf

Geant4 physics list, step

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi Ecole Polytechnique - LLR

The stepping:

- The stepping treats processes generically:
- The stepping does not know what processes it is Handling
- The stepping imposes on the processes to Cooperate in their AlongStep actions; Compete for PostStep and AtRest actions;
- Processes can optionally emit also a «signal» to require particular treatment:
 - notForced: «standard» case;
 - forced: PostStepDolt action is applied anyway;
 - conditionallyForced: PostStepDolt
 - applied if AlongStep has limited the step;

The stepping: Stepping Invocation Sequence of Processes for a particle travelling

- At the beginning of the step, determine the step length: Consider all processes attached to the current G4Track; Define the step length as the smallest of the lengths among: All AlongStepGetPhysicalInteractionLenght()., All PostStepGetPhysicalInteractionLength()
- Apply all AlongStepDoIt() actions, « at once »: Changes computed from particle state at the beginning of the step; Accumulated in the G4Step; Then applied to the G4Track, from the G4Step.
- Apply PostStepDolt() action(s) « sequentially », as long as the particle is alive: Apply PostStepDolt() of process which proposed the smallest step length;
 apply « forced » and « conditionally forced » actions

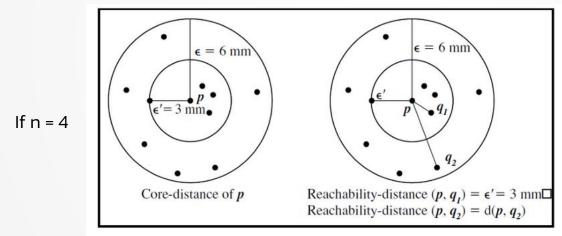
Geant4 physics list, step

Derived from CERN Geant4 User's Workshop November 11th–15th 2002, John Apostolakis, Marc Verderi At rest: Ecole Polytechnique - LLR

- I. If the particle is **at rest**, is stable and can'tannihilate, it is killed by the tracking:To be more accurate: if a particle at rest has no« AtRest » actions defined, it is killed.
- Otherwise determine the lifetime: Take the smallest time among: All AtRestGetPhysicalInteractionLenght() Called «physical interaction length» but returns a time!
- 3. Apply the AtRestDolt() action of the process which returned the smallest time.

OPTICS^{13,14} (Ordering points to identify the clustering structure)

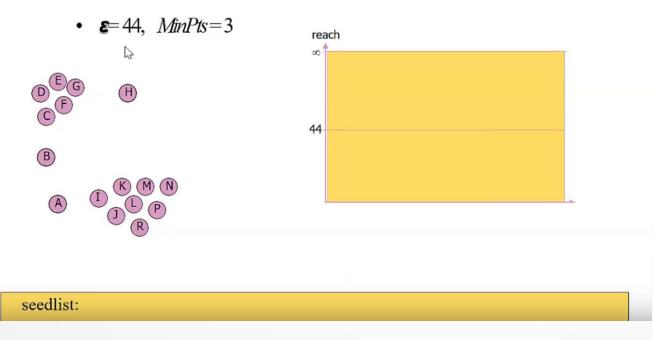
- n (number of neighbours): user input
- Core distance: The minimum distance to make a point a core point, so that it contains number of neighbours n
- Reachability-distance:
 - a. If point < the core-distance reachability distance = core-distance
 - b. If point > core-distance, reachability distance = distance between the point and core point



Ankerst, Mihael, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. "OPTICS: ordering points to identify the clustering structure." ACM SIGMOD Record 28, no. 2 (1999): 49-60.
Schubert, Erich, Michael Gertz. "Improving the Cluster Structure Extracted from OPTICS Plots." Proc. of the Conference "Lernen, Wissen, Daten, Analysen" (LWDA) (2018): 318-329.

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

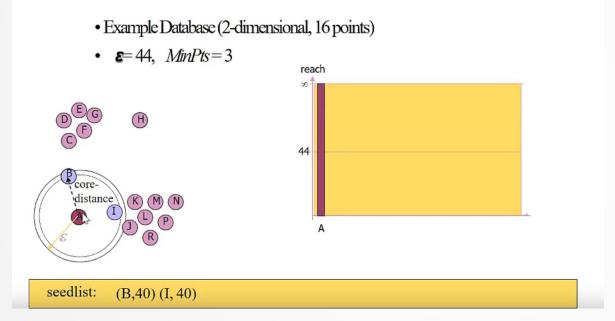
Optics algorithm takes the points in a certain order and assigns them properties.



Min neighbours:2

CERN, 14.06.2022

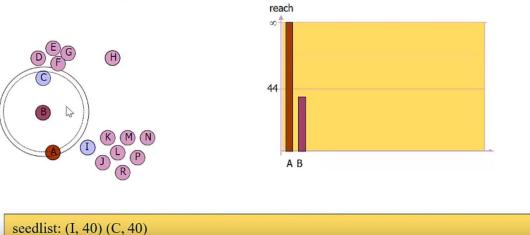
Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s



- A is the first point -> it's reachibility is infinite. (How far is the point from the last point?)
- B and C have are 40 units far away from A.

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

- Example Database (2-dimensional, 16 points)
- **E**=44, *MinPts*=3

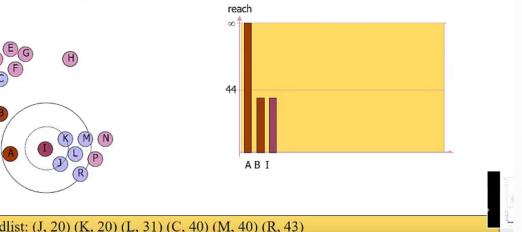


- Next point: B.
- Seedlist is updated and ordered by reachability.

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

• Example Database (2-dimensional, 16 points)





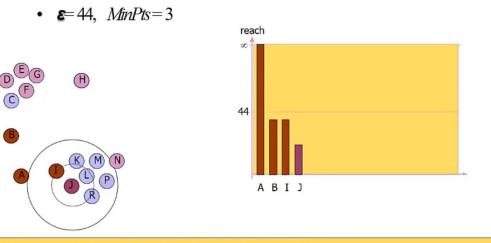
Next point I.

- The core distance is much smaller (K and J are close).
- The seedlist is updated and • ordered by reachability.

seedlist: (J, 20) (K, 20) (L, 31) (C, 40) (M, 40) (R, 43)

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

• Example Database (2-dimensional, 16 points)

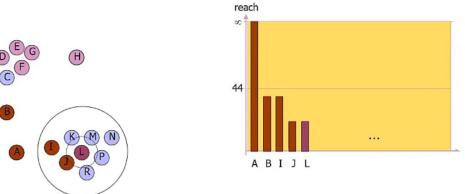


- Next point J
- The seedlist is updated and ordered by the rechability.

seedlist: (L, 19) (K, 20) (R, 21) (M, 30) (P, 31) (C, 40)

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

- Example Database (2-dimensional, 16 points)
- **E**=44, *MinPts*=3



- Next point L
- The seedlist is updated and ordered by the rechability.

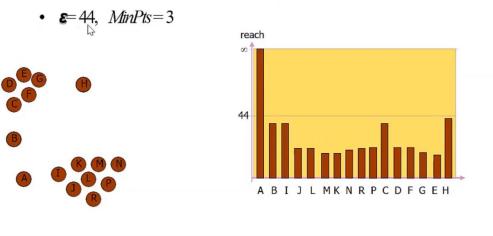
seedlist: (M, 18) (K, 18) (R, 20) (P, 21) (N, 35) (C, 40)

Min neighbours:2

CERN, 14.06.2022

Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

• Example Database (2-dimensional, 16 points)



• The valleys represent the clusters.

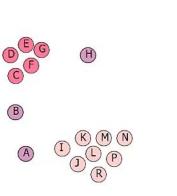
seedlist: -

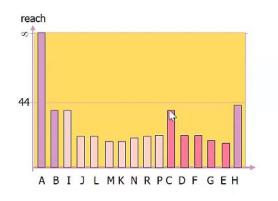
Min neighbours:3

CERN, 14.06.2022

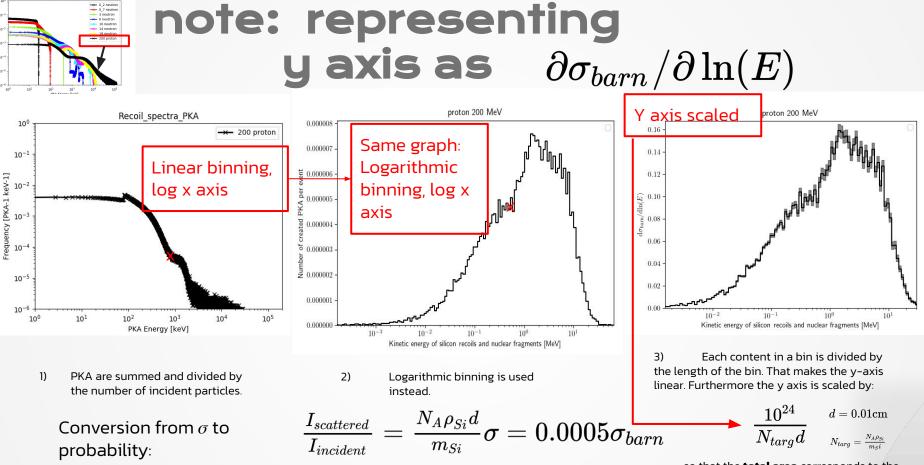
Explanation from: https://www.youtube.com/watch?v=CVOmWaHOTA8&t=133s

- Example Database (2-dimensional, 16 points)
- **E**=44, *MinPts*=3





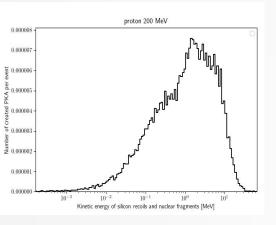
• The valleys represent the clusters.



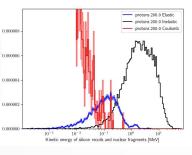
Recoil spectra all PKA

so that the **total area** corresponds to the **total cross section** of creating the PKA.

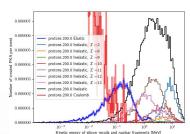
note: representing yaxis as $\partial E_{NIEL}/\partial \ln(E_{recoil})$



 PKA are summed and divided by the number of incident particles. Logarithmic binning is used instead, that makes the y axis linear. 2) PKA are divided into Elastic and Inelastic parts (Coulomb part is added from QGSP_BIC_HP_SS simulation). Inelastic part is further divided into different spectra according to the Z number.



3) Inelastic part is further divided into different spectra according to the Z number.



4) For Coulomb, Elastic and Inelastic Si, Al and Mg recoils a Lindhard formulation is used¹².

For a recoil silicon in a silicon lattice, they read as:

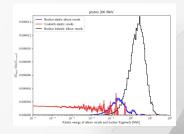
$$E_{\rm de} = \frac{E_{\rm Si}}{1 + k \times g(\epsilon)},\tag{2}$$

with $k=0.1462,\,\epsilon=1.014\times10^{-2}\times Z_{\rm Si}^{-7/3}\times E_{\rm Si}=2.147\times10^{-5}E_{\rm Si}$ and the universal function

$$g(\epsilon) = 3.4008 \times \epsilon^{1/6} + 0.40244 \times \epsilon^{3/4} + \epsilon \tag{3}$$

5) For alphas¹³, Xapsos-Burke values were used to calculate NIEL.

6) Each content in a bin is divided by the length of the bin so that the **total area** corresponds to the **total NIEL**.



12) Bergmann, Benedikt, et al. "Ionizing Energy Depositions After Fast Neutron Interactions in Silicon." IEEE Transactions on Nuclear Science, vol. 63, Aug. 2016, pp. 2372–78. NASA ADS, <u>https://doi.org/10.1109/TNS.2016.2574961</u>

13) Xapsos, M.A. & Burke, E.A. & Badavi, F.F. & Townsend, Lawrence & Wilson, John & Jun, I. (2005). NIEL calculations for high-energy heavy ions. Nuclear Science, IEEE Transactions on. 51. 3250 - 3254. 10.1109/TNS.2004.839136.