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

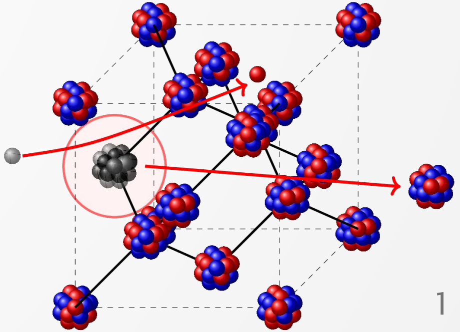
NIEL(non-ionizing energy loss)

Simulations and displacement damage studies towards a more complex NIEL concept for radiation damage modelling and prediction,

Queen Mary University of London

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

Previous RD50 contribution:
https://indico.cern.ch/event/1157463/contributions/4922734/



41st RD50 Workshop, 29.11.2022

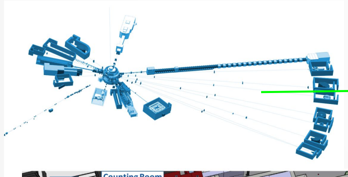
CONTENTS

The NIEL hypothesis & motivation for this study

NIEL (non-ionizing energy loss)

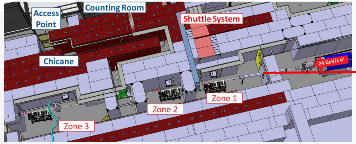
- **NIEL** is a physical quantity describing the non-ionizing energy loss as the particle travels through the medium.
- The amount of **NIEL** can be correlated to the ammount of radiation damage (NIEL scaling model) and therefore to predict the life time of the detectors.
- **NIEL** is usually expressed as an equivalent to **NIEL** of 1 MeV neutrons. (put in 95 MeV mb)

ESS



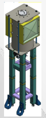
neutrons

IRRAD



protons

GIF++



gamma-rays

- **NIEL scaling assumption is** **used by the LHC experiments and beyond**
- **Long term goal:** revisit the damage factors stated by different irradiation facilities and used by the experiments.

NIEL (non-ionizing energy loss)

$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT$$

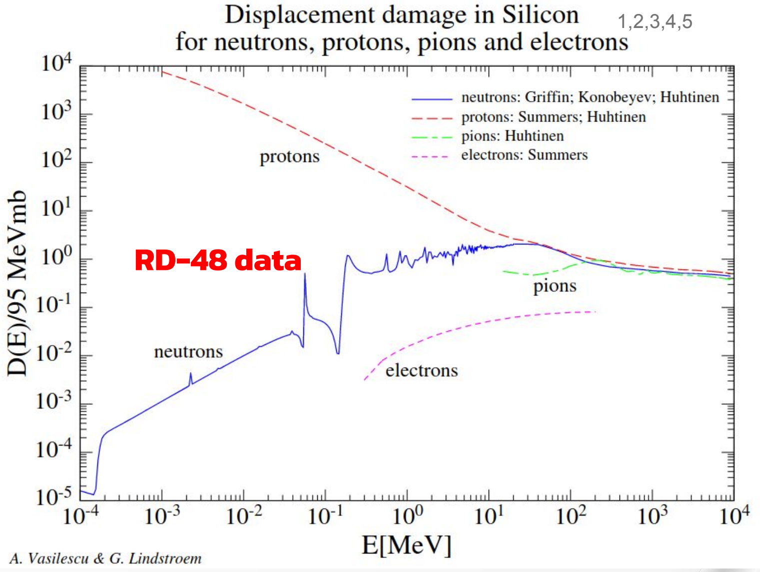
- **T_0**: energy of incident particle
- **T**: energy transferred to the recoil atom
- **(dσ/dT)**: differential partial cross section for a particle with energy **T_0** to create a recoil atom with energy **T** in the i-th reaction
- **Q(T)**: partition factor giving the fraction of **T** that is going into further displacements
- **N_A** : Avogadro number
- **A :** atomic mass of target atom

Displacement damage function

$$NIEL(T_0) = \frac{N_A}{A} D(T)$$

MeV cm²/g

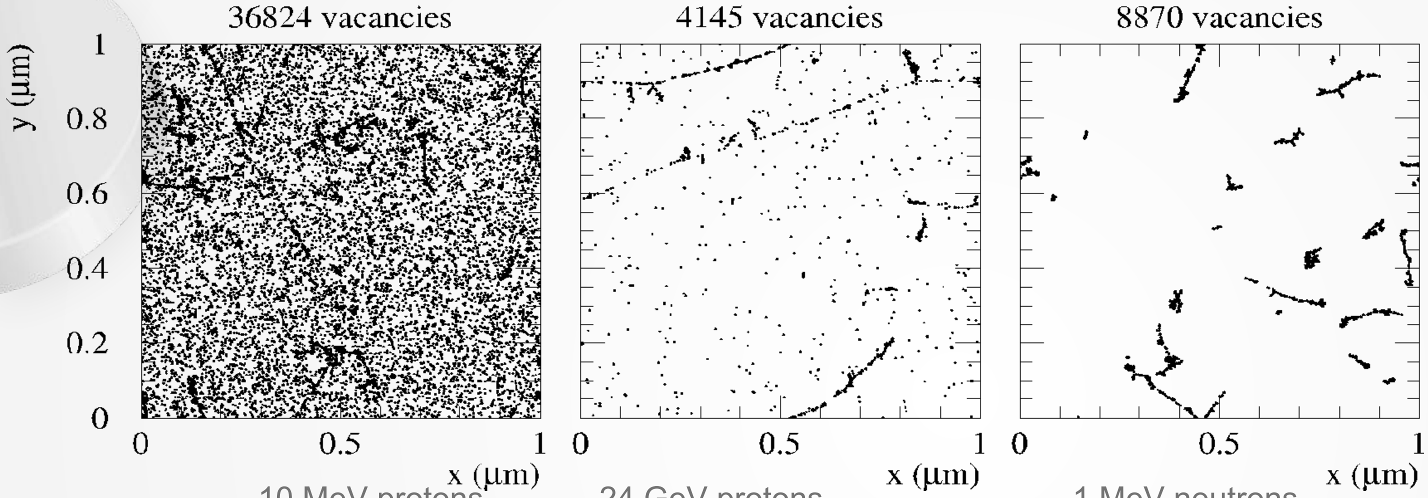
MeV mb



1) Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg), https://rd50.web.cern.ch/niel/
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.
4) 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.
5) 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.

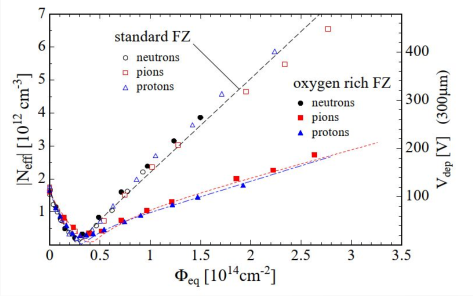
Revisiting NIEL

Simulations of radiation damage by M. Huhtinen[6].

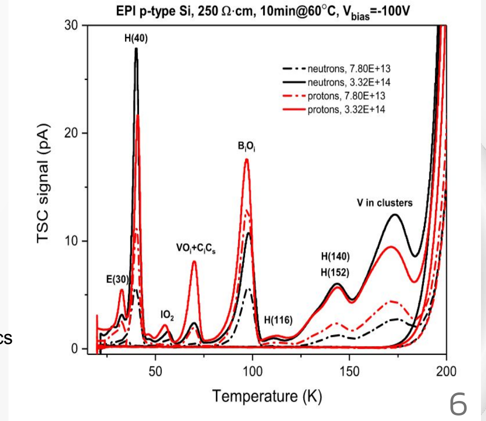


10 MeV protons   24 GeV protons   1 MeV neutrons

CERN RD48 : oxygen enriched silicon sensors[7].



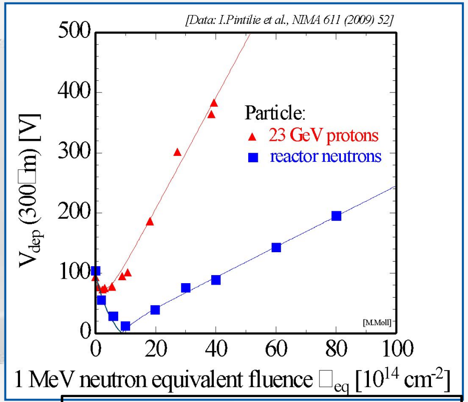
Radiation Damage in P-Type EPI Silicon Pad Diodes Irradiated with Protons and Neutrons[8].

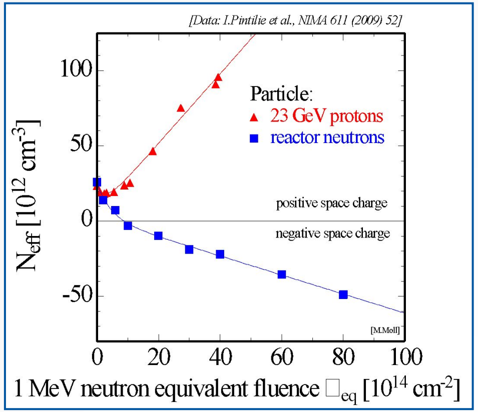


- NIEL doesn't distinguish between cluster and point displacement, i.e. the same displacament energy has a very different distribution of damage on the microscopic level.
- NIEL scaling violation reported in oxygen enriched silicon samples (CERN RD-48, Vdep (Φeq) dependence on particle type), differences between neutron's and proton's damage.

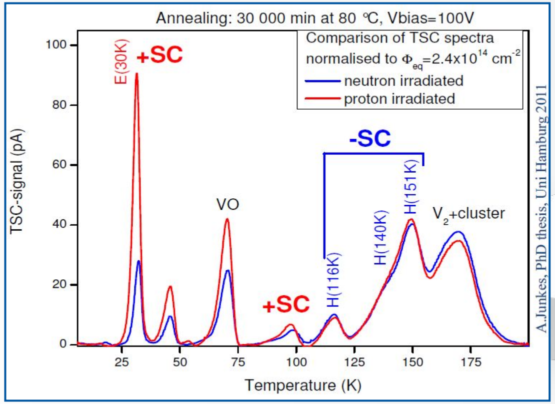
6) Huhtinen, M. “Simulation of Non-Ionising Energy Loss and Defect Formation in Silicon.” Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 491, no. 1, Sept. 2002, pp. 194–215. ScienceDirect, https://doi.org/10.1016/S0168-9002(02)01227-5.
7) G. Lindström et al., Nucl. Instrum. Meth. A466 (2001) 308, doi:10.1016/S0168-9002(01)00560-5.
8)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.

Revisiting NIEL



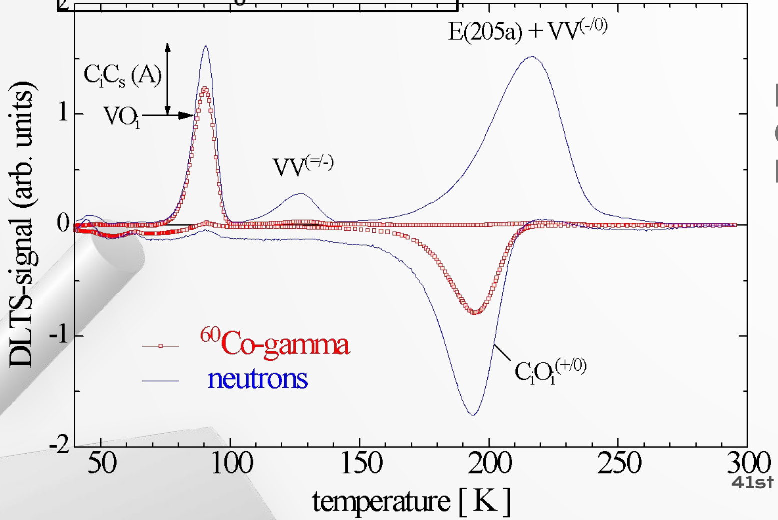


$$V_{dep} = \frac{q_0}{\epsilon\epsilon_0} \cdot |N_{eff}| \cdot d^2$$



Protons: no space charge inversion

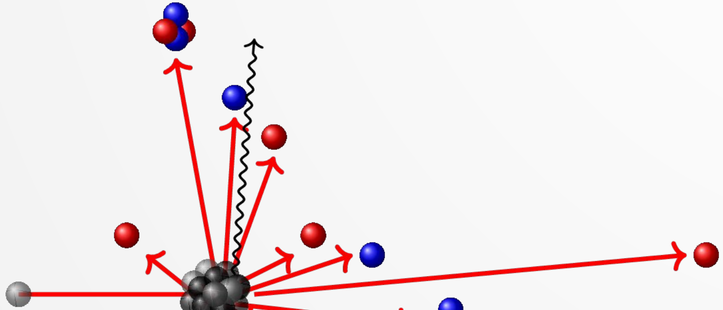
Neutron: space inversion

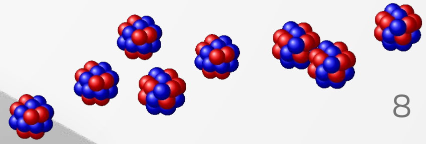


From the microscopic perspective: (DLTS measurement)
Gamma irradiation: only point defects
Neutron irradiation: cluster and point defects

Therefore the aim of this study is to **partition NIEL function into cluster contribution and point defects contribution**.

Geant4 simulations of atomic displacements





Geant4 simulation framework

Geant4[9,10](for GEometry ANd Tracking) is a Monte Carlo simulation platform for the passage of particles through matter.

Define a geometry:

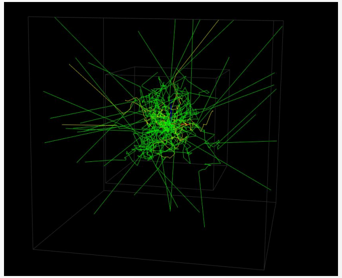
For most of the simulations:
1mm x1 mm x100 µm

Choose a physics list:

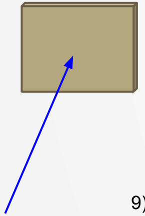
1. For PKA (Primary knocked-on atoms):
   a. *QGSP_BERT_HP* (Nuclear scattering)
   b. *QGSP_BERT_HP__SS* (Coulomb scattering)
2. For SDC (Subsequent displacement cascades)
   a. *Custom PhysicsList*[11]

Launch a simulation:

QGSP_BERT_HP
QGSP_BERT_HP__SS
Custom Physics[11]



Define a beam profile:

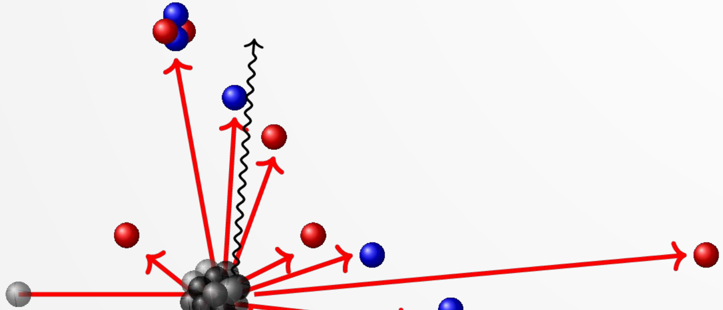


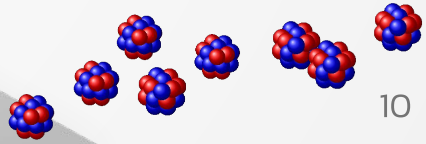
1. For PKA: Monochromatic pencil beam of protons and neutrons of various energies.
2. For SDC: Single Si particles of various energies being injected

Analyze (c++, python)

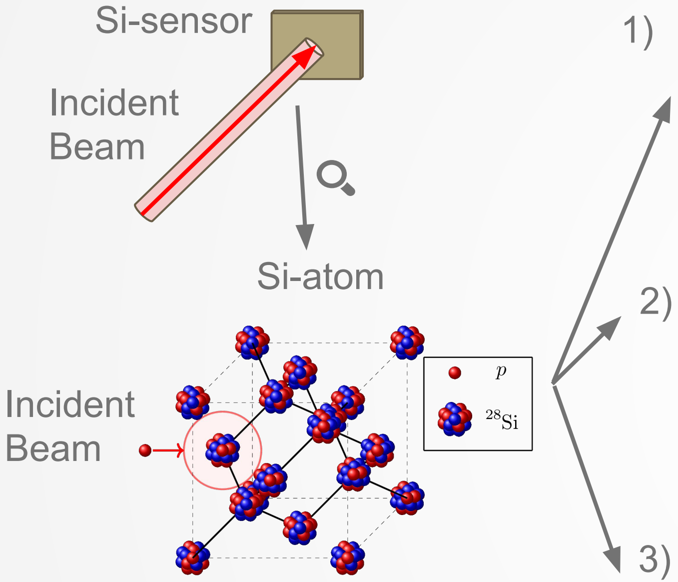
9) Agostinelli, S., et al. “Geant4—a Simulation Toolkit.” Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, D Detectors and Associated Equipment, vol. 506, no. 3, July 2003, pp. 250–303. ScienceDirect, https://doi.org/10.1016/S0168-9002(03)01368-8.
10) Allison, 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.
11) 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)

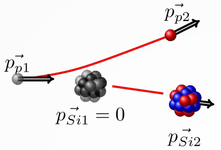




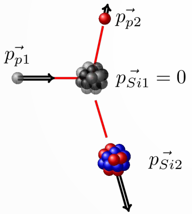
PKA cross section example



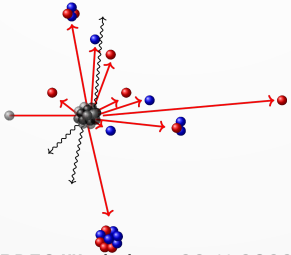
1) Coulomb elastic scattering (only charged particles)



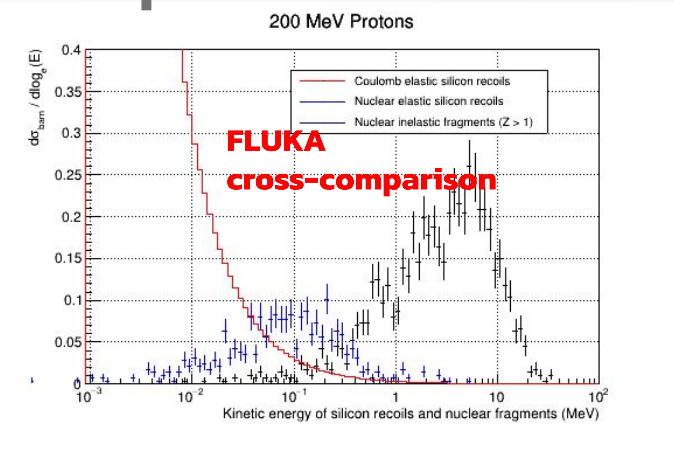
2) Nuclear elastic scattering

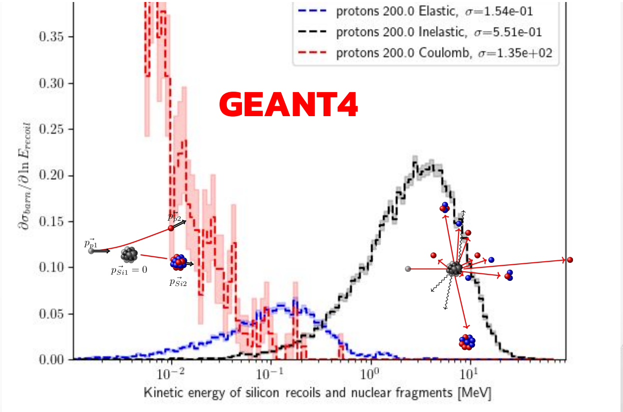


3) Nuclear inelastic scattering



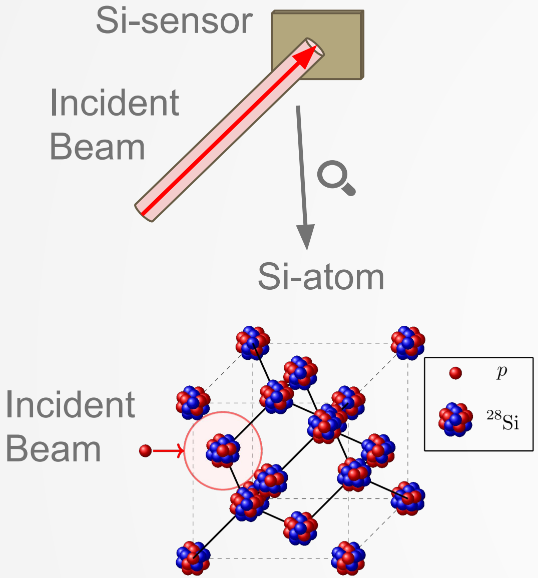
$$NIEL(T_0) = \frac{N_A}{A} \sum_i \int_{T_{min}}^{T_{max}} Q(T)\, T \left(\frac{d\sigma}{dT}\right)_i dT$$



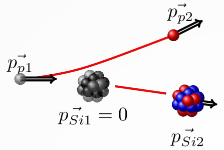


Area below the curve corresponds to the cross section. Displacement threshold = **21 eV**.

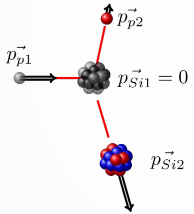
PKA cross section example



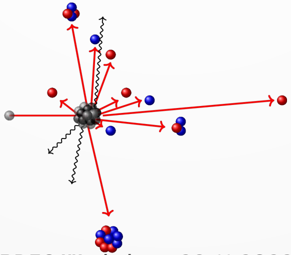
1) Coulomb elastic scattering (only protons)



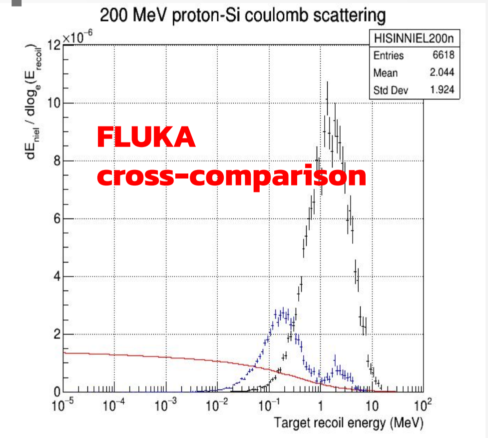
2) Nuclear elastic scattering

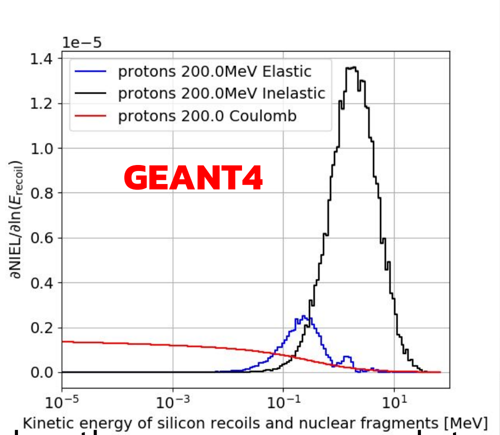


3) Nuclear inelastic scattering



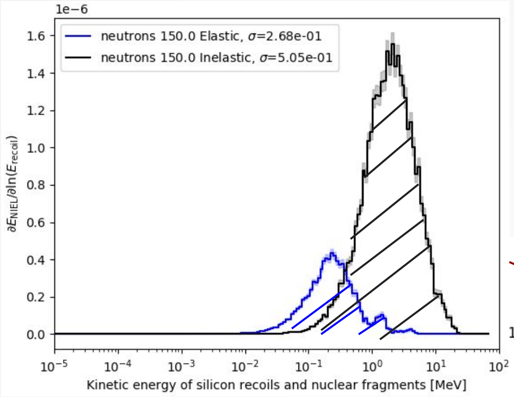
$$NIEL(T_0) = \frac{N_A}{A}\sum_i \int_{T_{min}}^{T_{max}} Q(T)T\left(\frac{d\sigma}{dT}\right)_i dT$$



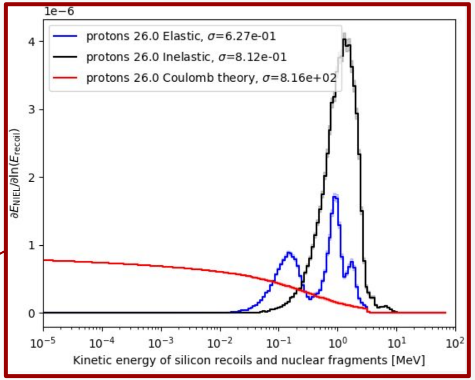


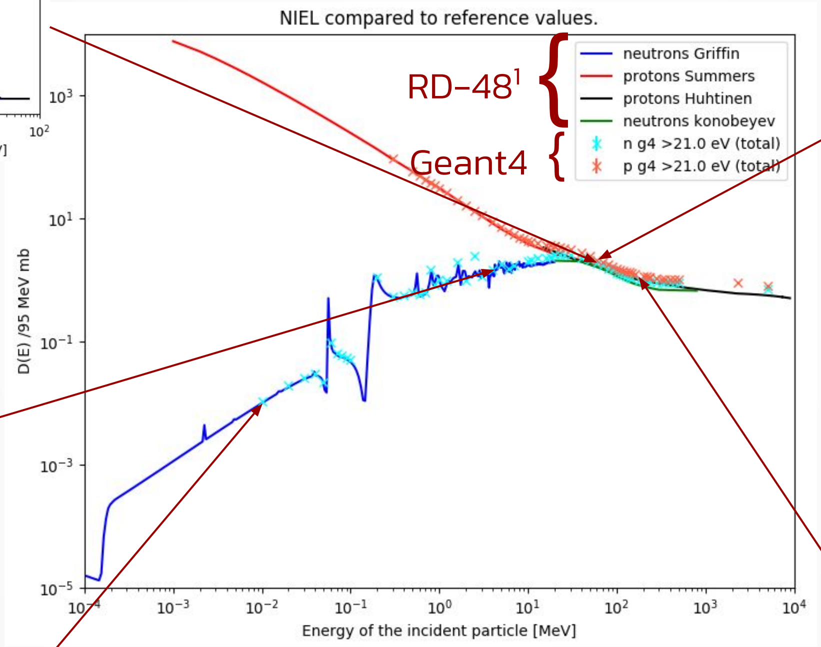
Area below the curve corresponds to the NIEL for respective reaction.

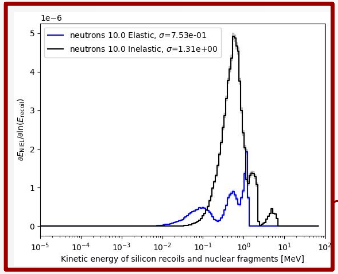
Producing NIEL curves

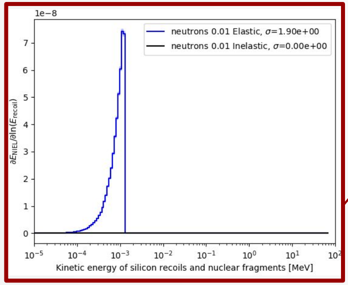


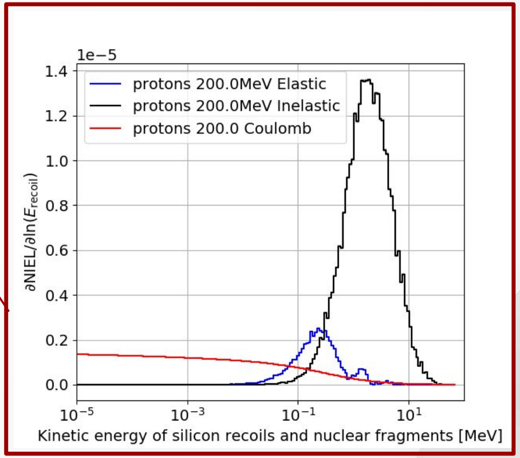
- Integrating the recoil spectra above threshold displacement energy (21 eV) yields 1 point on the NIEL curve



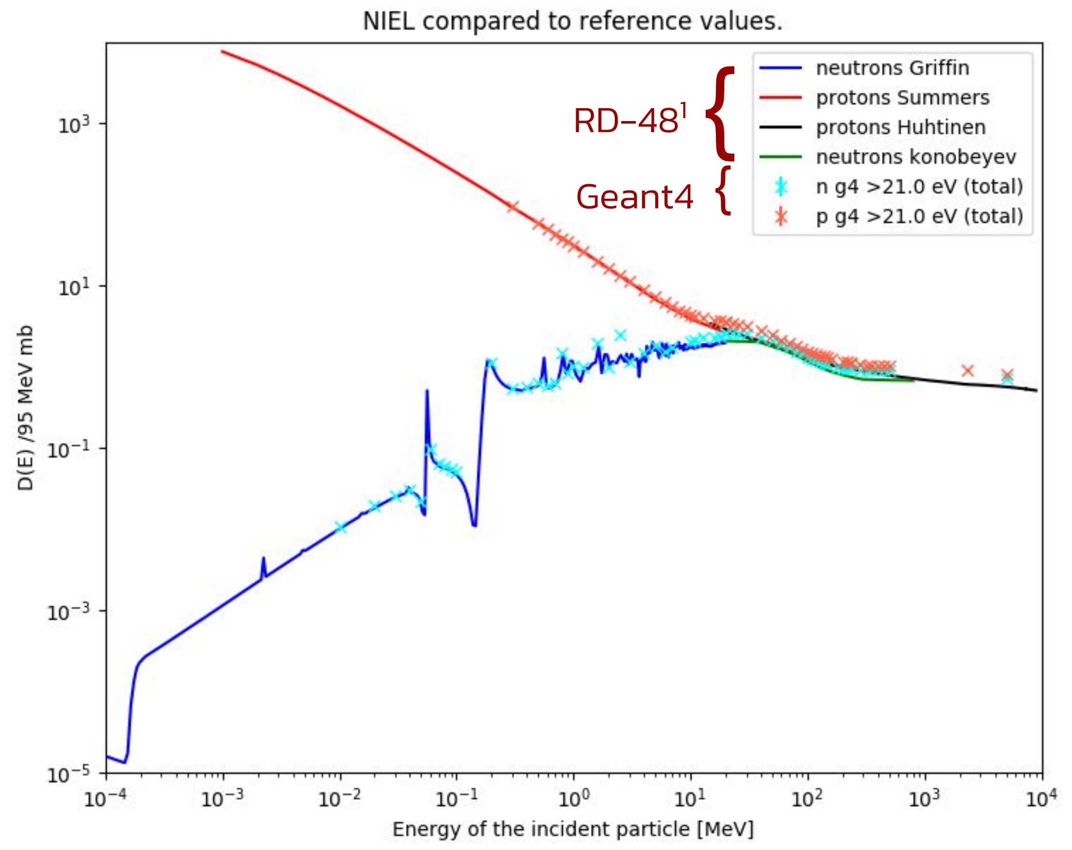








Producing NIEL curves



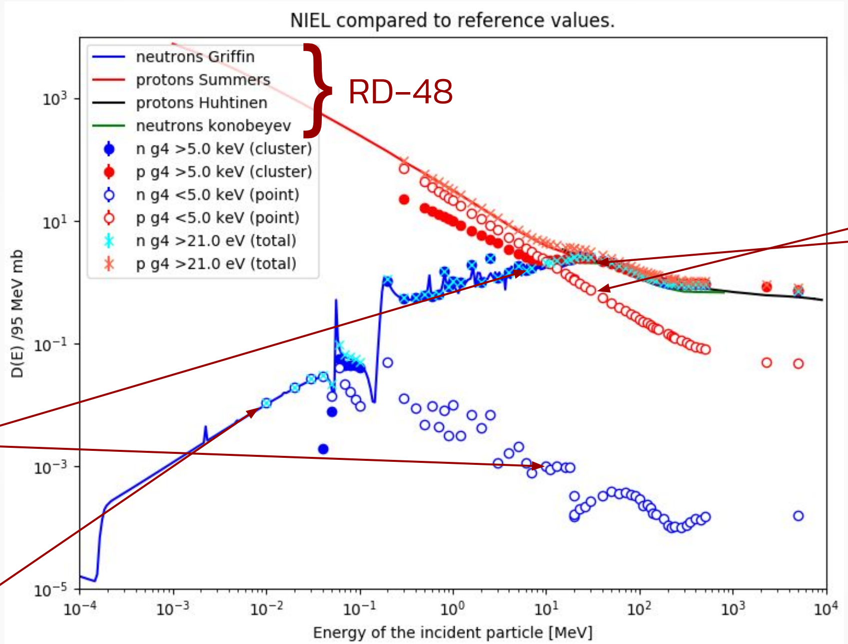
- Good agreement with the previous data (RD-48)
- Gives confidence in the used approach.

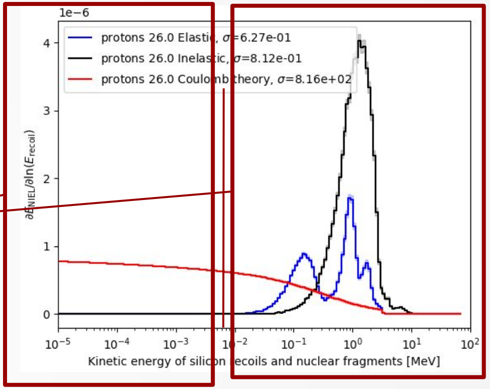
1) Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg), https://rd50.web.cern.ch/niel

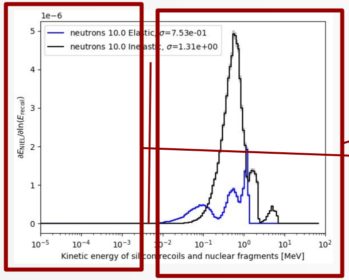
How to divide NIEL into clustered/isolated defects?

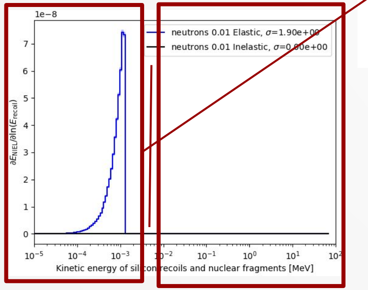
Initial approach :
Use threshold (from the literature) for cluster formation

- Recoils < 5 keV: point displacements
- Recoils > 5 KeV: point displacements+ cluster displacements



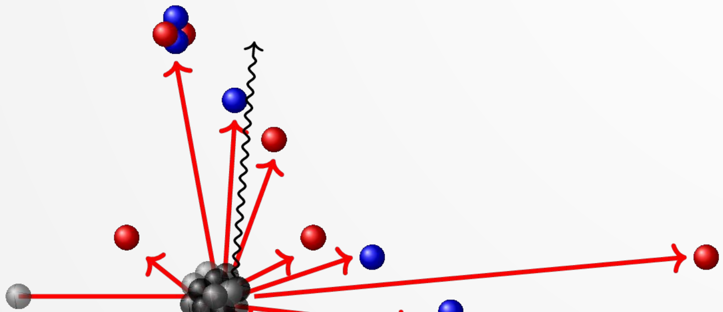






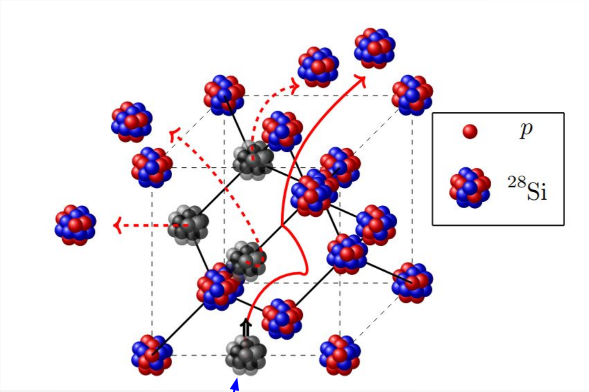
- Good as initial approach
- Not clear which part of the >5 keV is point-defects and which part is the cluster defect

Secondary recoils and atomic cascades

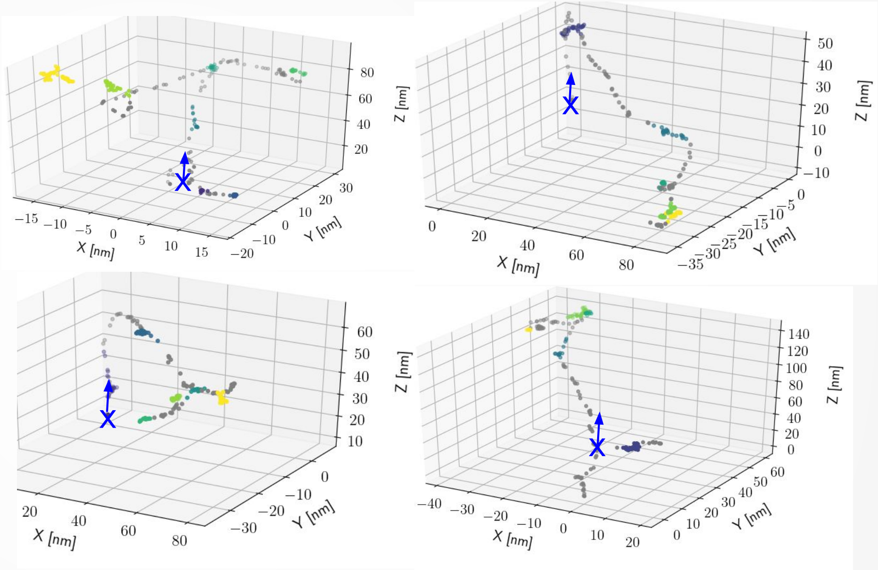


Secondary recoils and atomic cascades

- Geant4 studies with Screened Nuclear Recoil process[11]
- Focus on the propagation of Si-recoil in Silicon (no incident beam)



1 Si injected

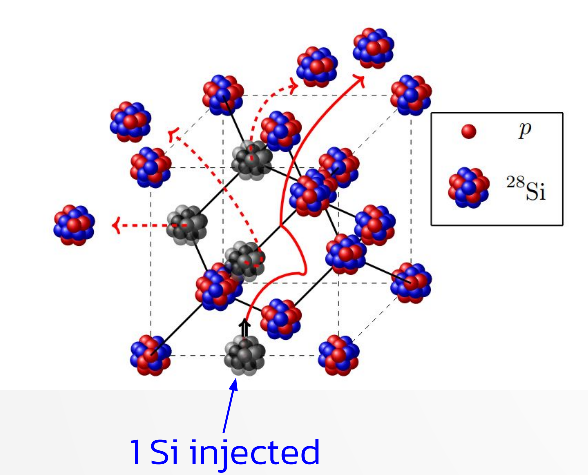


X: PKA 100 keV Si injected (0,0,0) with momentum along the positive z direction

11) 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.

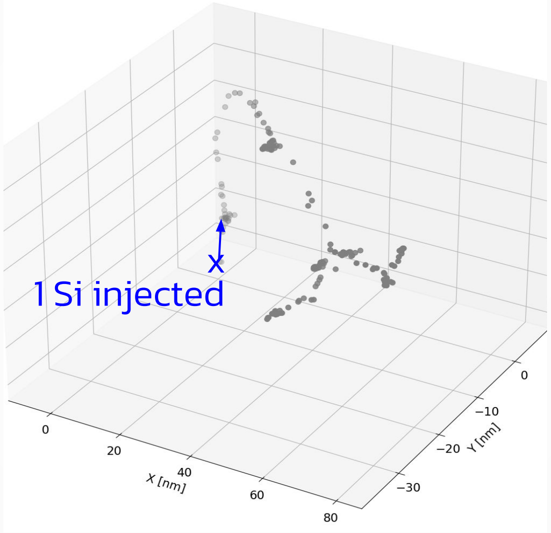
How to define a cluster? What algorithm to choose?

- Geant4 studies with Screened Nuclear Recoil process[11]
- focus on the propagation of Si-recoil in Silicon (no incident beam)

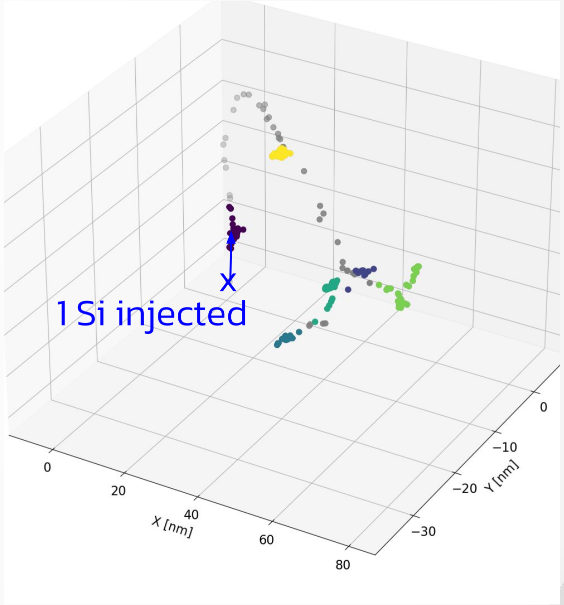


Example:

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

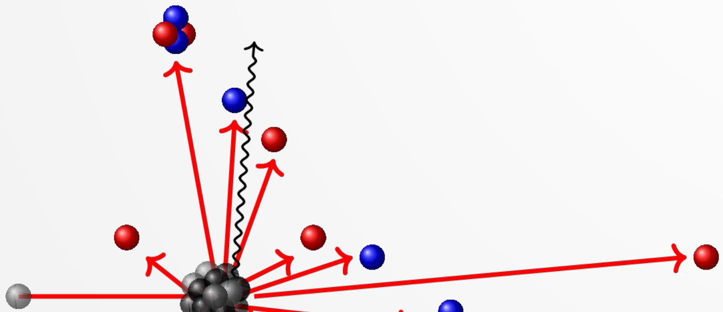


Grey dots: isolated displacements
Colored dots: clustered displacements

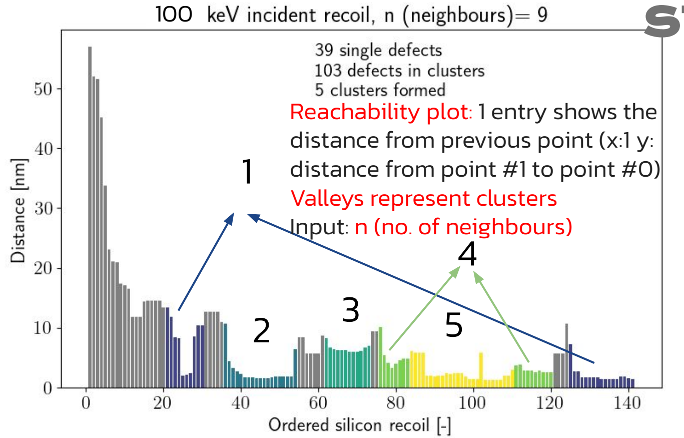


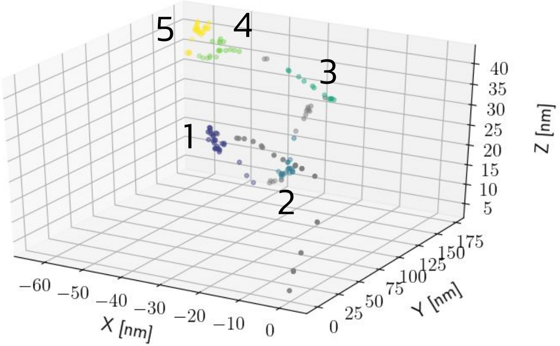
11) Raine, Melanie, et al. “Simulation of Single Particle Displacement Damage in Silicon - Part I: Global Approach and Primary Interaction Simulation.” IEEE Transactions on Nuclear Science, vol. 64, no. 1, Oct. 2016, pp. 133–40. HAL Archives Ouvertes, https://doi.org/10.1109/TNS.2016.2615133.

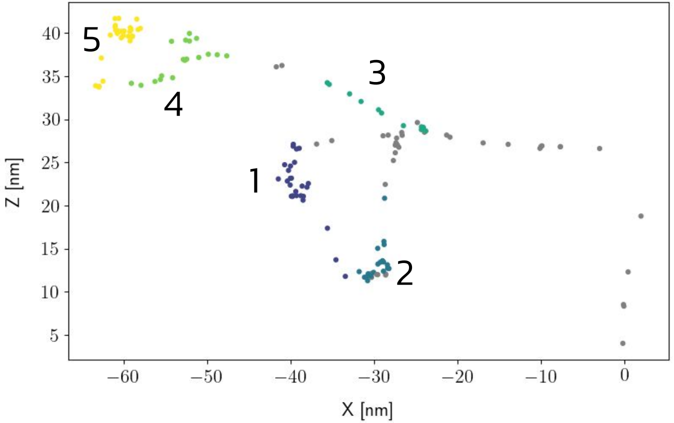
Isolated versus cluster defects



OPTICS[15,16] (Ordering points to identify the clustering structure)

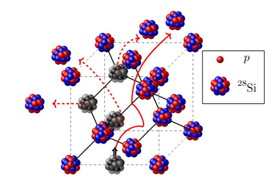






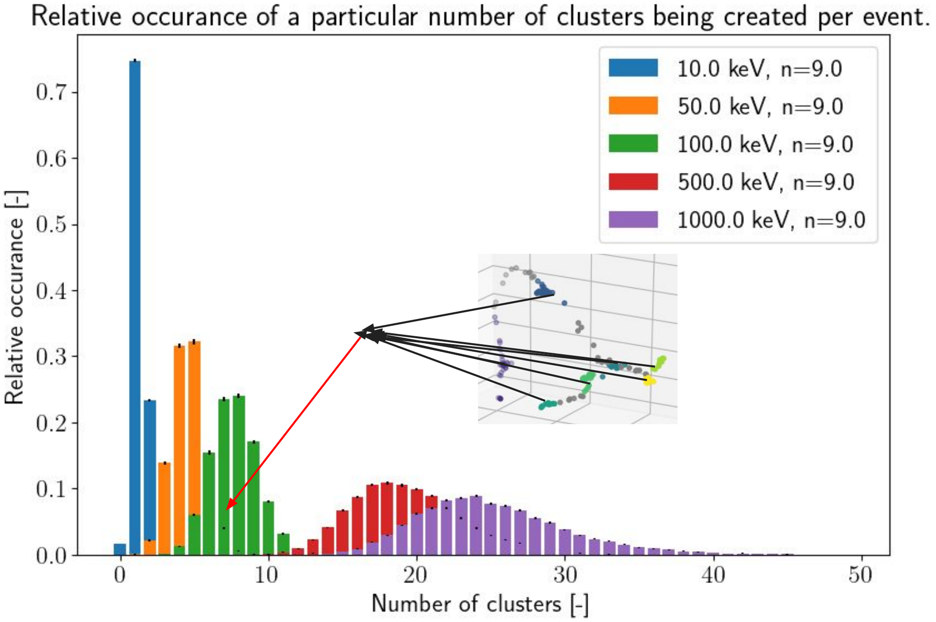
- Algorithm flow explain in the Appendix (Slide 34)
- Basic idea:
  - Ordering points and plotting their distances produces **Reachability plot**
  - Valleys in the reachability plot represent clusters
- Algorithm needs a user input: minimum number of samples to create cluster

15) 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.
16) Schubert, Erich, Michael Gertz. “Improving the Cluster Structure Extracted from OPTICS Plots.” Proc. of the Conference “Lernen, Wissen, Daten, Analysen” (LWDA) (2018): 318-329.
17) https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s tutorial



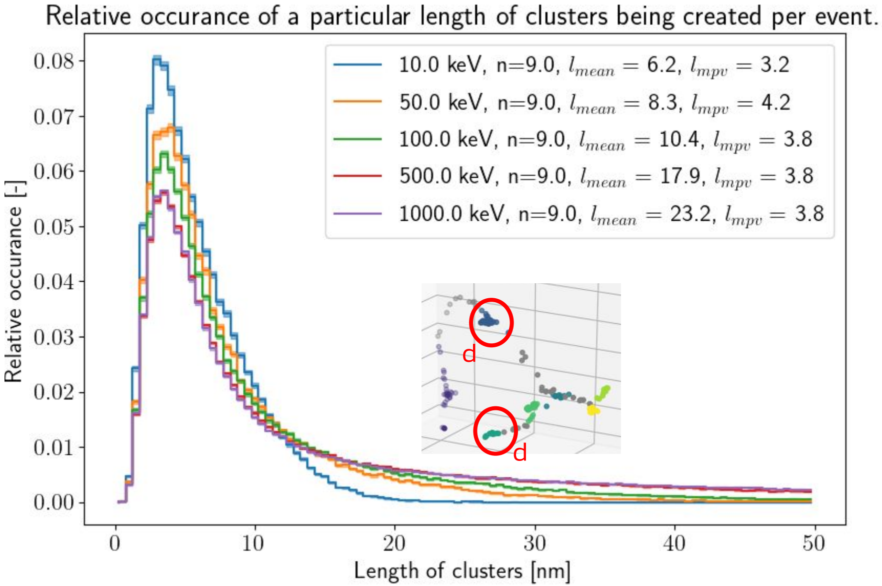
RESULTS (Si recoil input)

How many clusters?



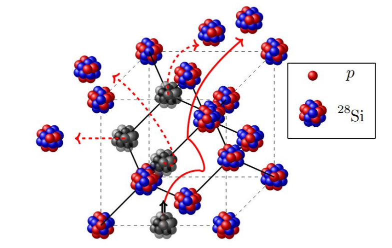
How large are the clusters?

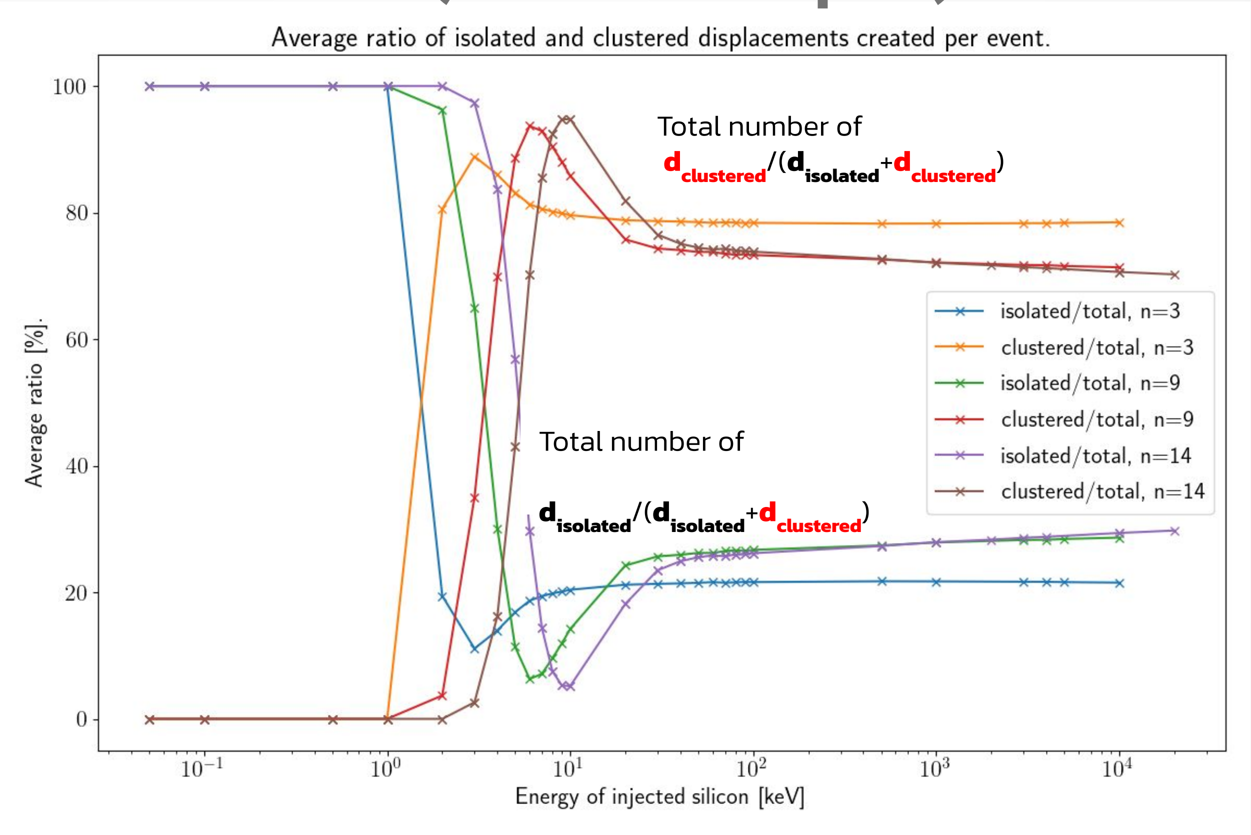
Length := diameter of the smallest enclosed sphere around the cluster



- 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.

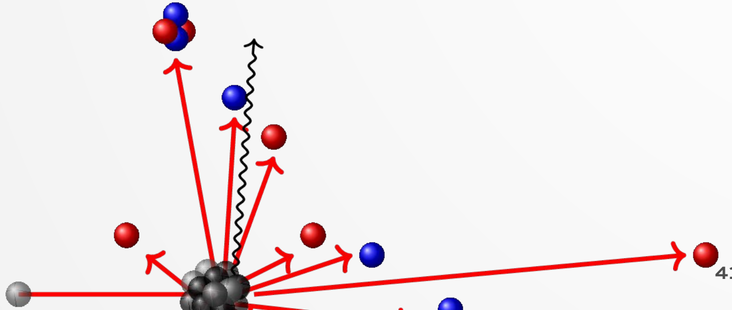
RESULTS (Si recoil input)

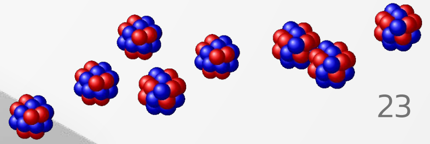




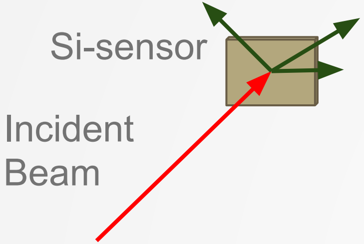
- For E > 50 keV stable ratio of point-like and cluster displacements are independen the choice of n
- The threshold energy for creatir stable ratio of point-like and cluster displacements depends on the algorithm parameter.

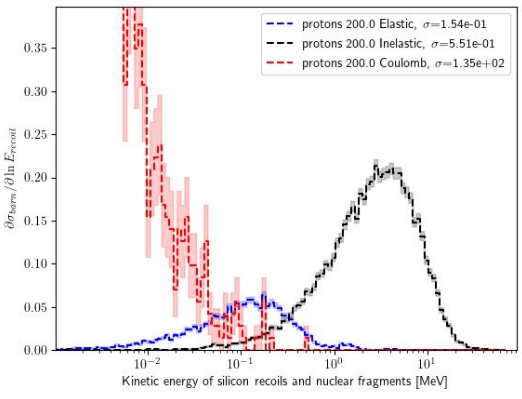
Atomic displacements produced by high-energy particles

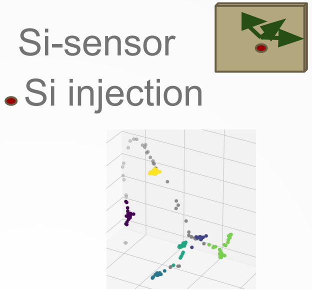


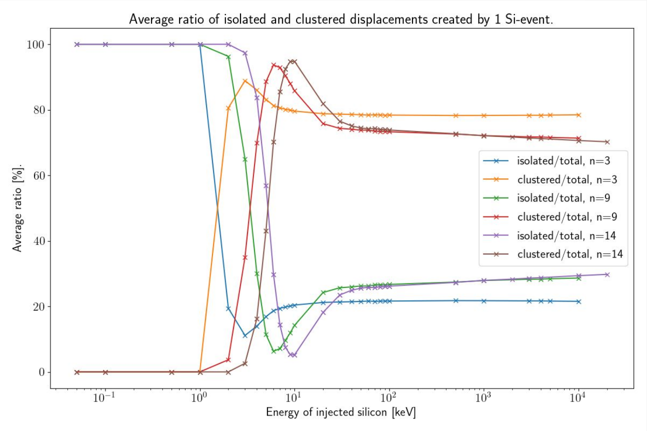


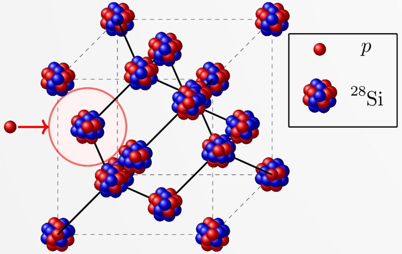
Displacements produced by high-energy particles



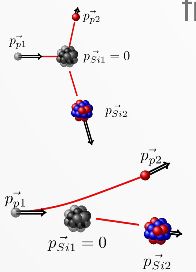


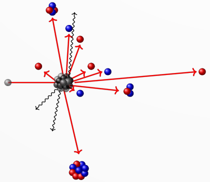




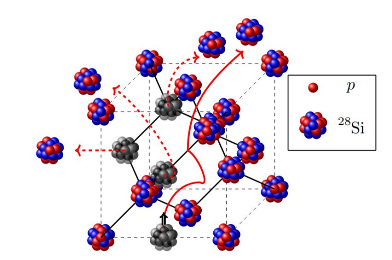


1) PKA characterized
   a) Saved in raw file.



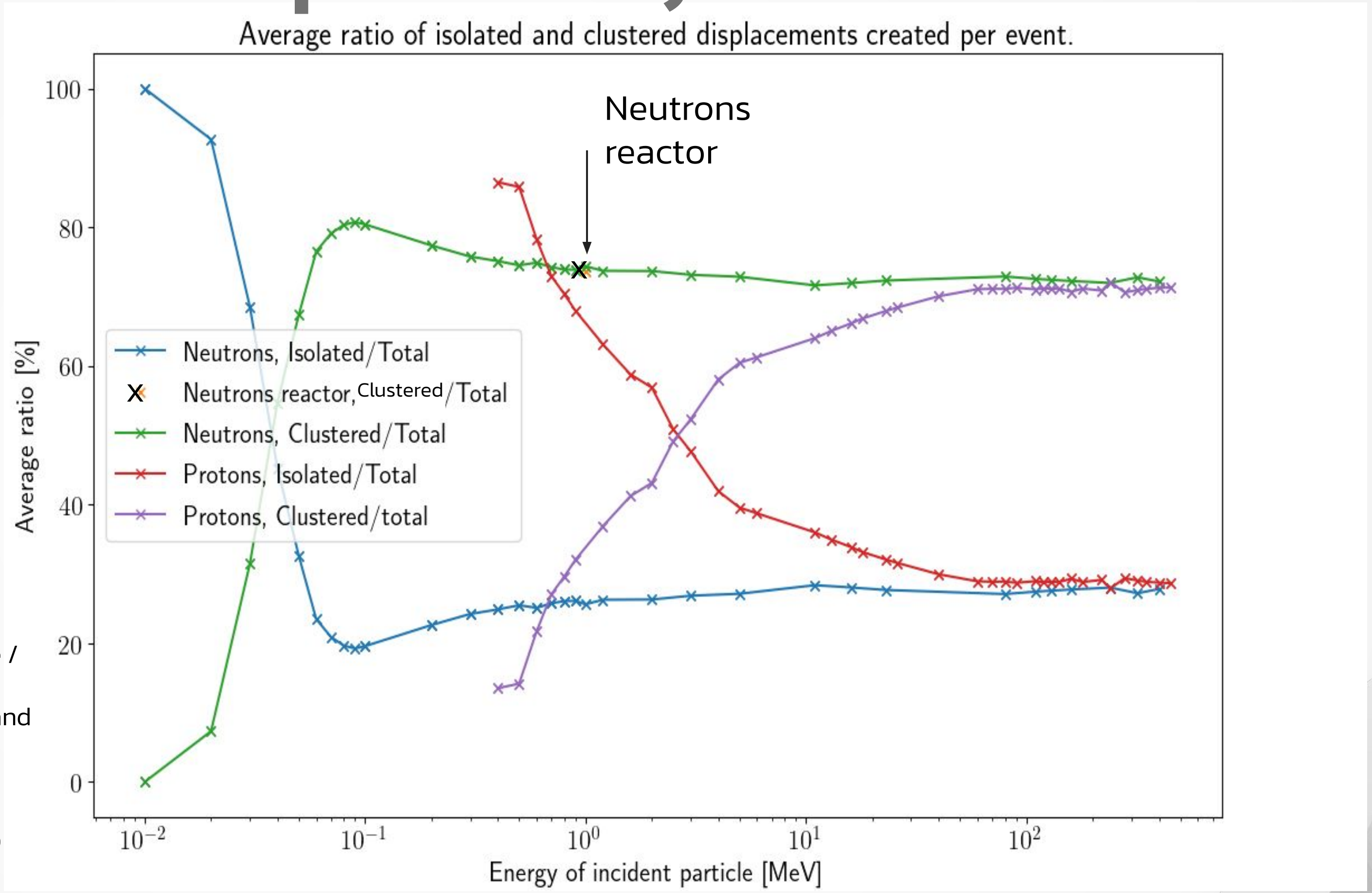


2) Subsequent Si cascade (SKA):
   a) The raw PKA output used as an input for SKA
   b) SKA generated
   c) OPTICS algorithm applied on the generated SKA



RESULTS: protons, neutrons

Results for n number of neighbours = 9, xi =0.05 (parameter from 0-1, steepness of the valleys on the reachability plot)



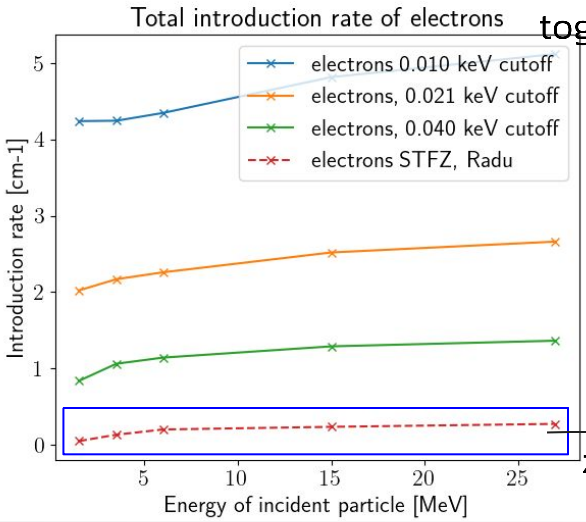
- For E > 0.1 MeV stable ratio of point-like and cluster displacements for neutrons
- For E> 100 MeV stable ratio of point-like and cluster like displacements for protons.
- E > 100 MeV ratio of cluster-like / point-like defects (or cluster/ isolated) ~ 70/30 similar for p and n irradiation
- point-like defects dominant for low particle E (< 0.1 MeV for neutron, < 100 MeV for protons)

Work in-progress

Electron induced damage

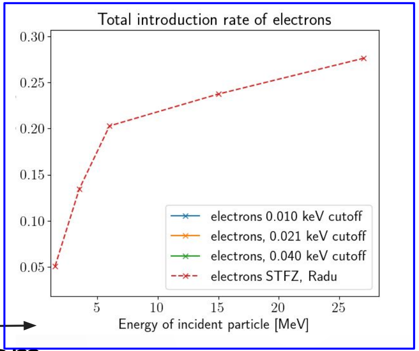
Work in-progress

VOi, V3 and V2 together

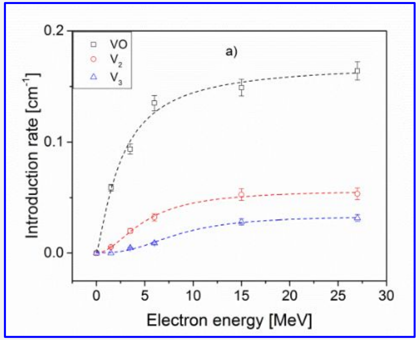


zoom

Total introduction rate from Radu is approx 10 ~ lower.



- The aim is to tune the parameters by using the measured values that we know.
- We would like to compare the total introduction rates and the rates between clustered and point defects.
- Tuning might depend on n, xi, cutoff limit.
- One of the options for the fine tuning would be to use a different constant for the processes that create only 1 PKA (a) and processes that create many SKA afterwards



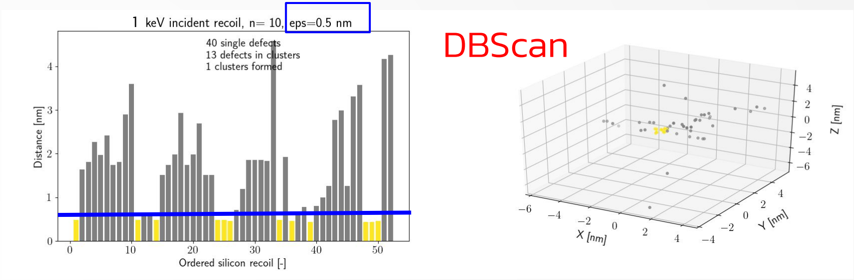
R. Radu: Bulk radiation damage in silicon:
from point defects to clusters

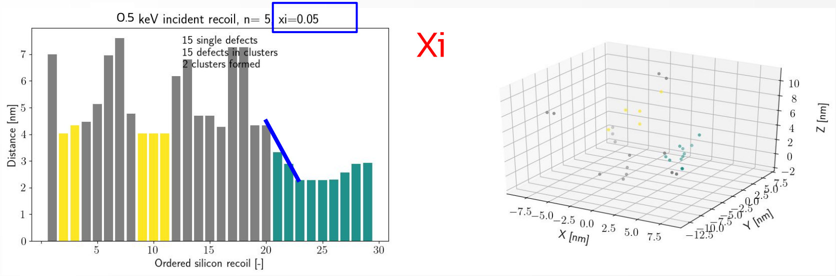
Tuning of the cluster model parameters

Method:

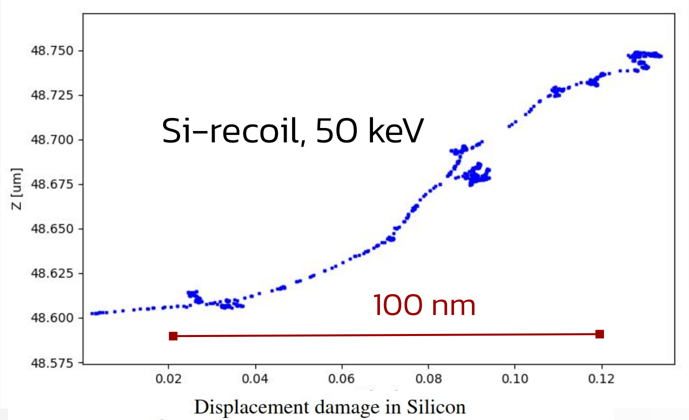
- Optics (number of samples, xi: steepness parameter)
- DBScan (number of samples, eps: extraction parameter)
    - The idea for DBScan could be to set eps=0.47 nm (2x interatomic distance) in order to be considered a cluster
    - The number of neighbours could be tuned by
        - <1-2 keV 0 clusters
        - <12 keV 1 cluster
        - >20 keV stable ratio of clusters and single displacements

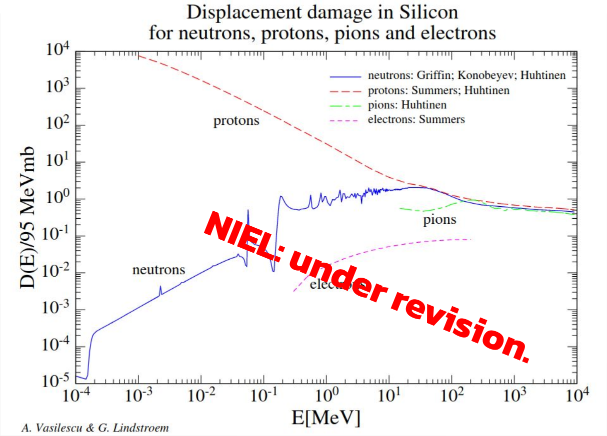
1





Outlook & next steps





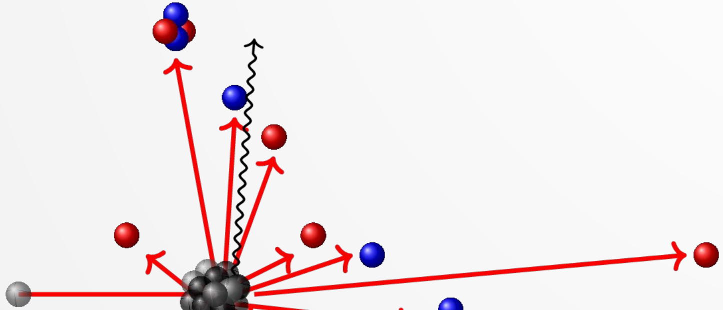
1) Data from A. Vasilescu (INPE Bucharest) and G. Lindström (Univ. of Hamburg), https://rd50.web.cern.ch/niel/

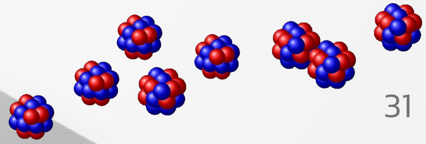
- Geant4 and FLUKA-based simulations have been carried out to produce NIEL curves.
- NIEL curves from literature (RD-48[1]) were successfully reproduced.
- Several cluster-finding algorithms have been tested to establish differences between different particles and particle energies.
  - First promising datasets from protons and neutrons shown in this presentation.
- Ongoing work:
  - Systematic studies on OPTICS with parameter tuning.
  - Studies and comparisons with the literature (cluster sizes, differences between vacancies and interstitials,...).
  - Separation of the NIEL curves into cluster and isolated displacements NIEL.
  - Extending studies to electrons and gammas.
  - Benchmarking with the experimental data in terms of defect introduction rates.
  - Comparison to other simulations (TRIM, kinetic monte-carlo, molecular dynamics, quasi-chemical).

THANKS!

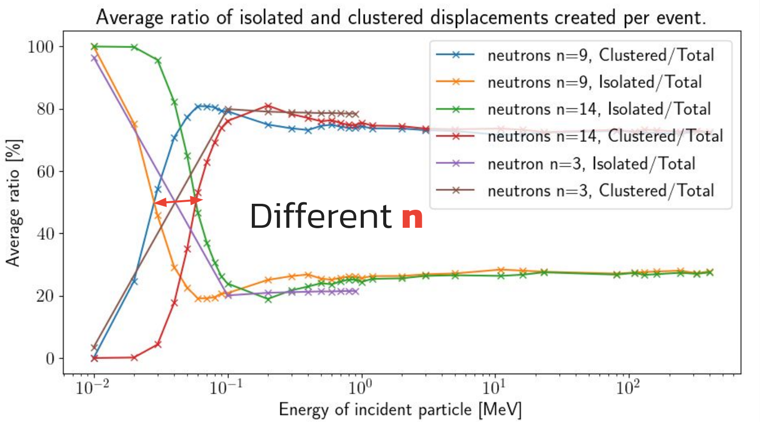
Do you have any questions?

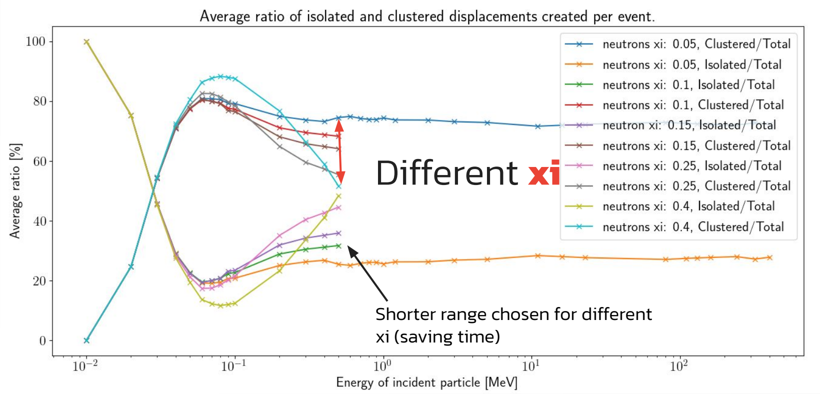
Extra slides

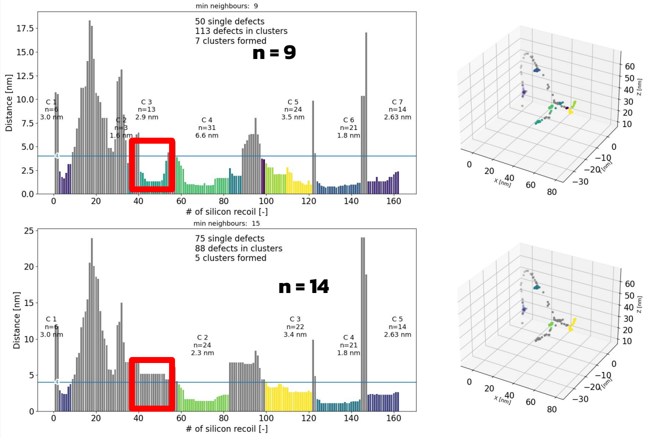




Paramater tuning: neutrons

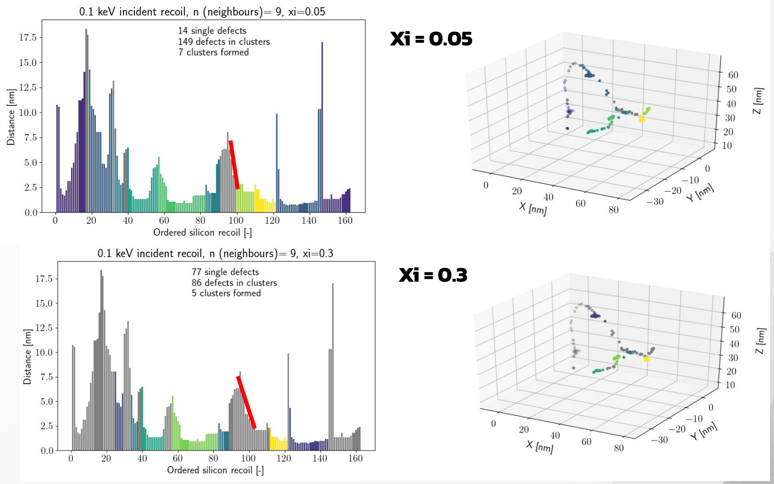






For the total ratio of Clustered vs isolated defects:

- n seems to shift the curve horizontally
- xi shifts the constant value the ratio eventually reaches.



Deeper explanation of the parameters:
https://scikit-learn.org/stable/modules/generated/sklearn.cluster.OPTICS.html
https://dl.acm.org/doi/pdf/10.1145/304181.304187

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: PostStepDoIt action is applied anyway;
  - conditionallyForced: PostStepDoIt
  - applied if AlongStep has limited the step;

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

1. 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()
2. 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.
3. Apply PostStepDoIt() action(s) « sequentially », as long as the particle is alive: Apply PostStepDoIt() of process which proposed the smallest step length;

apply « forced » and « conditionally forced » actions

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

At rest:

1. 1. 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.
2. Otherwise determine the lifetime: Take the smallest time among: All AtRestGetPhysicalInteractionLenght() Called «physical interaction length» but returns a time!
3. Apply the AtRestDoIt() action of the process which returned the smallest time.

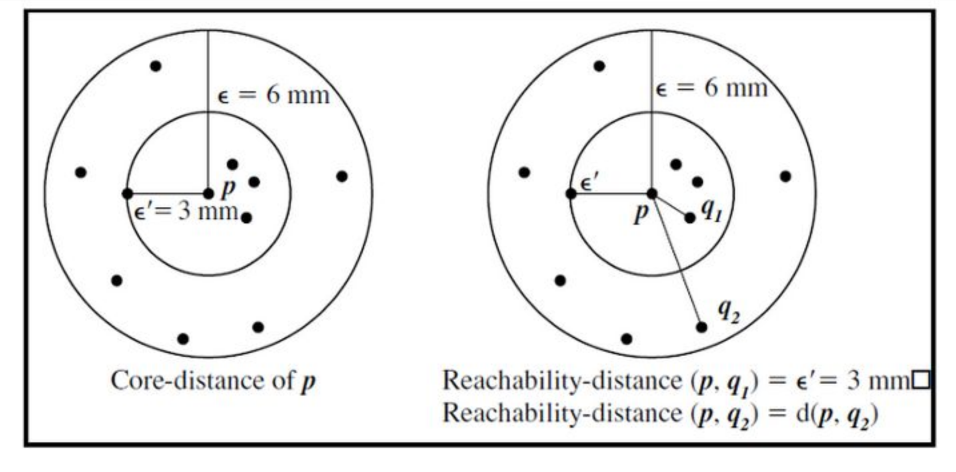
8) https://geant4.web.cern.ch/sites/default/files/geant4/collaboration/workshops/users2002/talks/lectures/PhysicsProcessesInGeneral.pdf

OPTICS[15,16] (Ordering points to identify the clustering structure)

Important concepts:

- **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

If n = 4

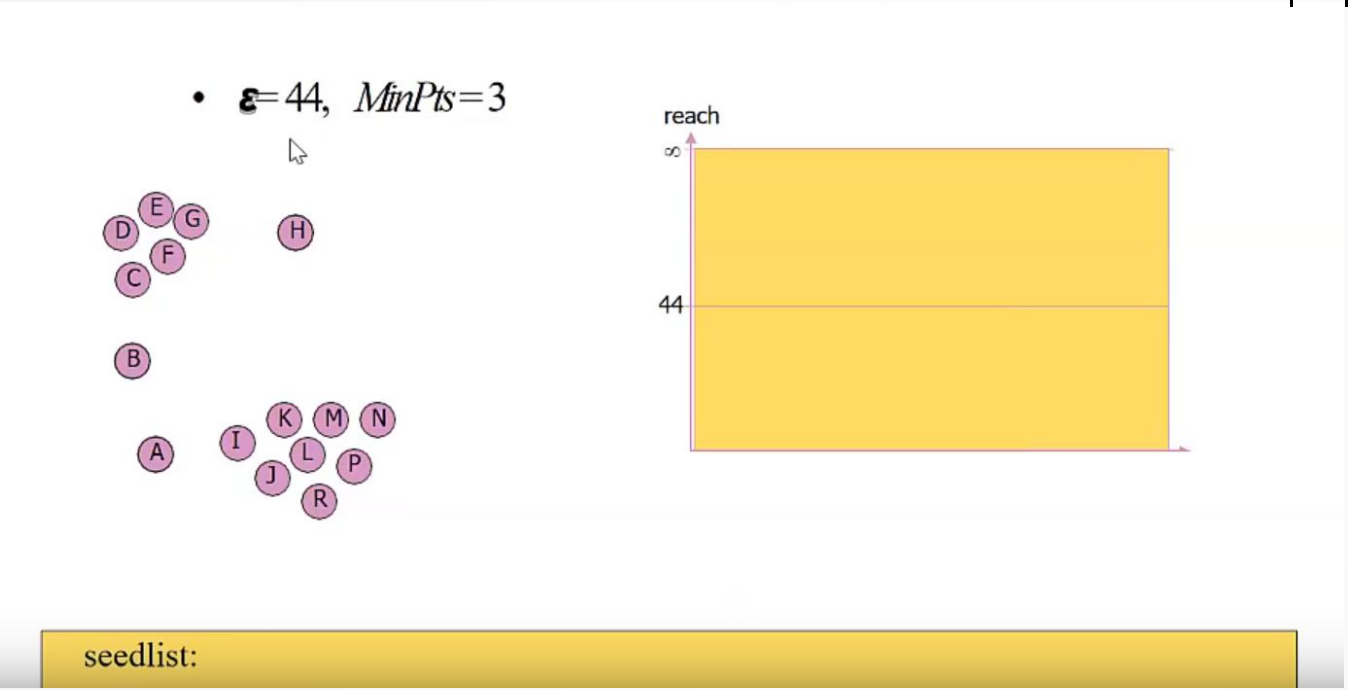


15) Ankerst, Mihael, Markus M. Breunig, Hans-Peter Kriegel, and Jörg Sander. “OPTICS: ordering points to identify the clustering structure.” ACM SIGMOD Record 28, no. 2 (1999): 49-60.
16) Schubert, Erich, Michael Gertz. “Improving the Cluster Structure Extracted from OPTICS Plots.” Proc. of the Conference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

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

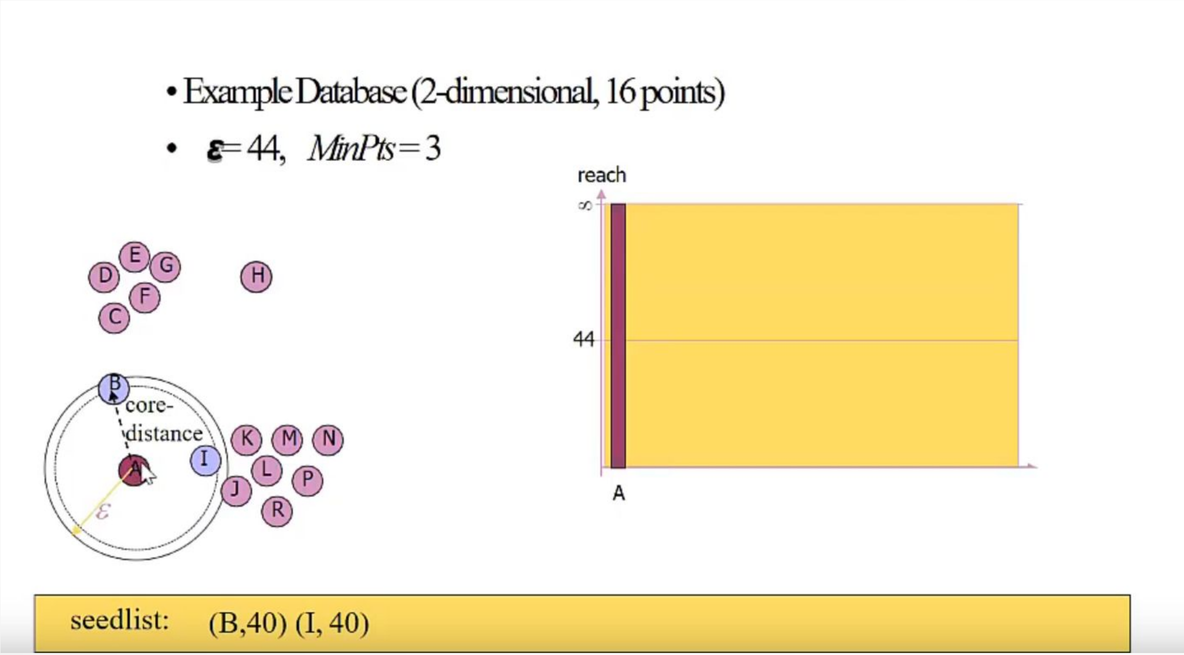
Optics algorithm takes the points in a certain order and assigns them properties.



Min neighbours:2

OPTICS

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

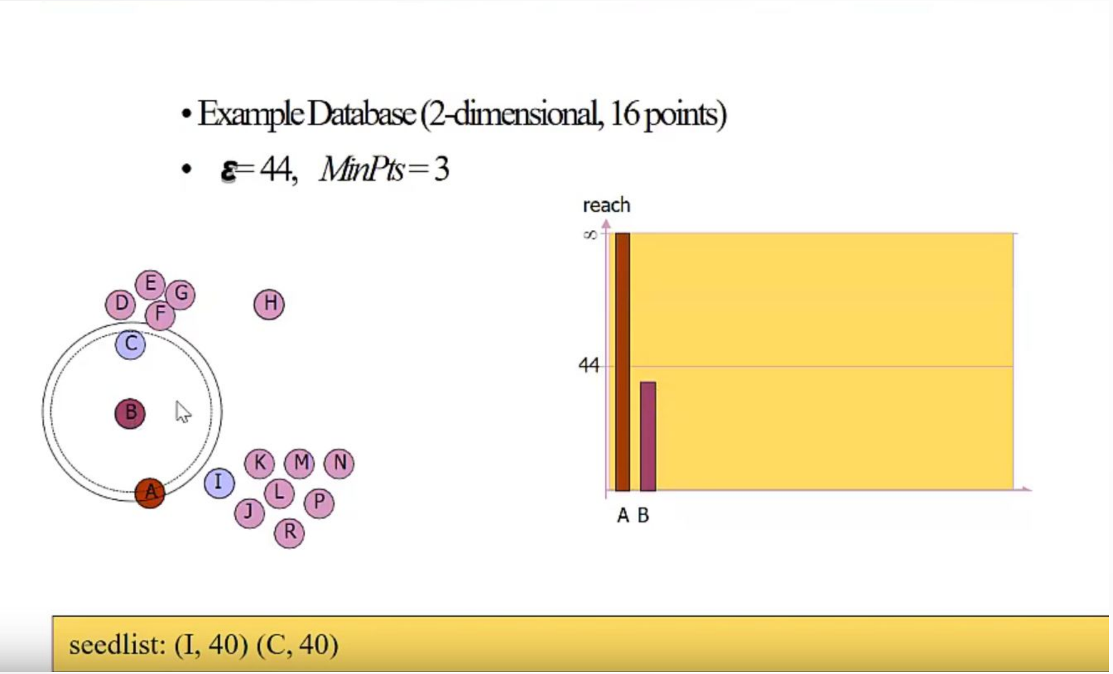


- A is the first point -> it's reachibility is infinite. (How far is the point from the last point?)
- B and C have are 40 units far away from A.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

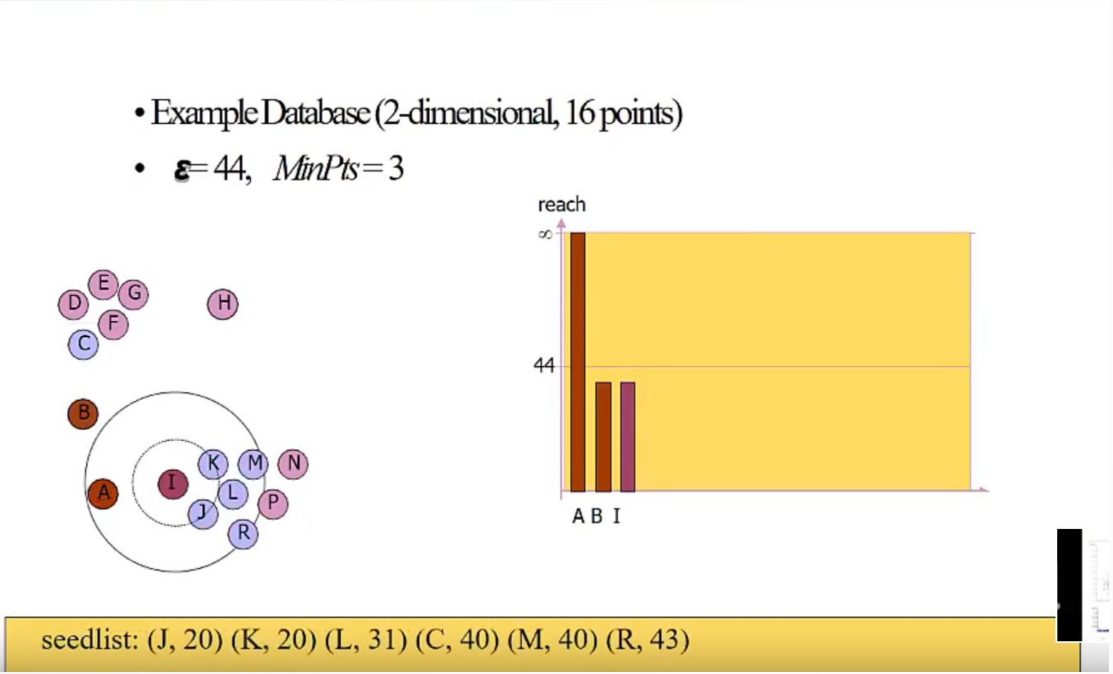


- Next point: B.
- Seedlist is updated and ordered by reachability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

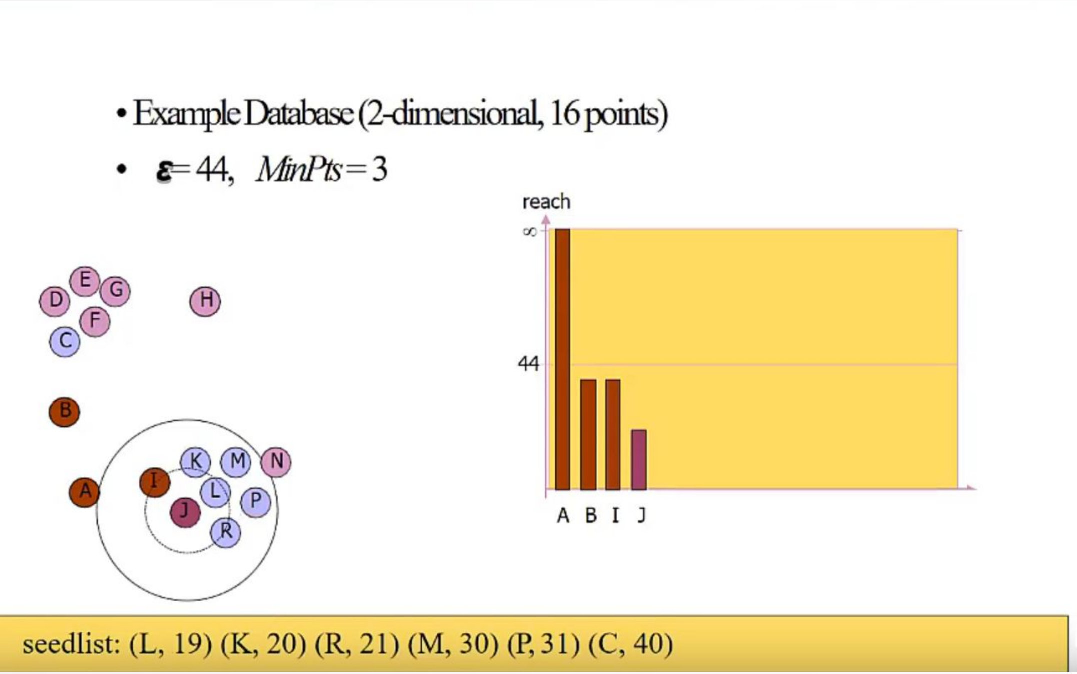


- Next point I.
- The core distance is much smaller (K and J are close).
- The seedlist is updated and ordered by reachability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

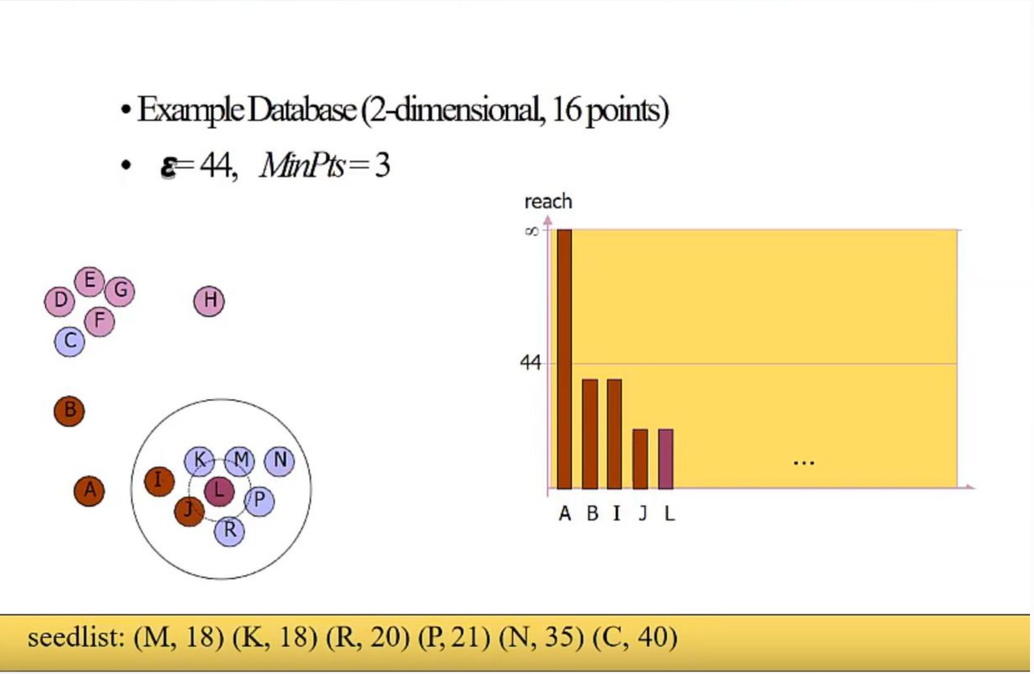


- Next point J
- The seedlist is updated and ordered by the rechability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

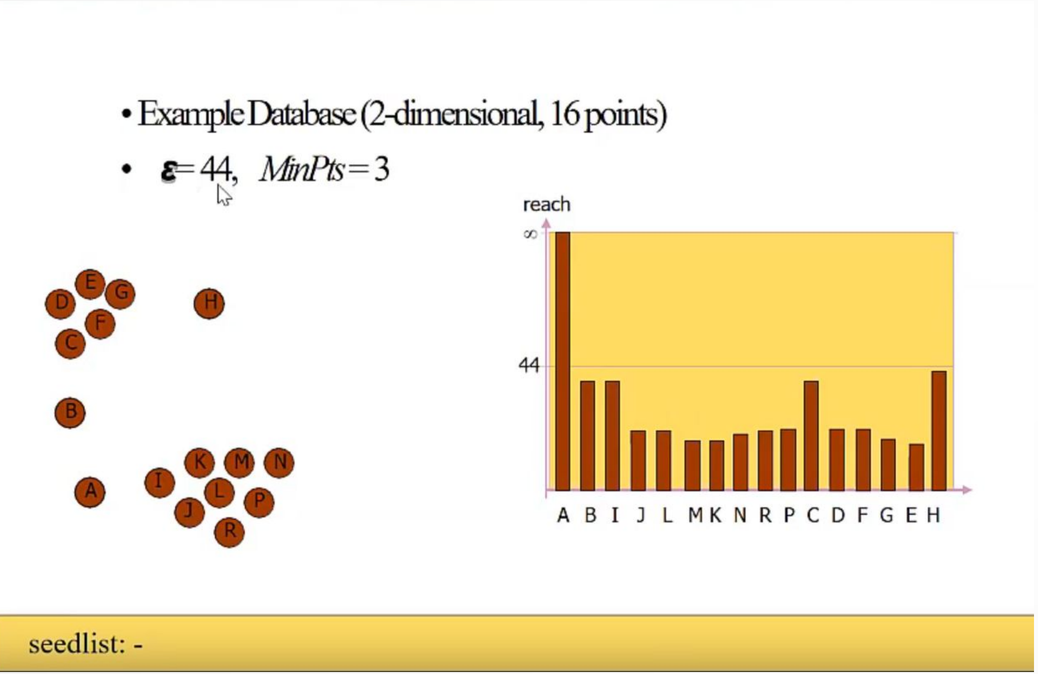


- Next point L
- The seedlist is updated and ordered by the rechability.

Min neighbours:2

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s

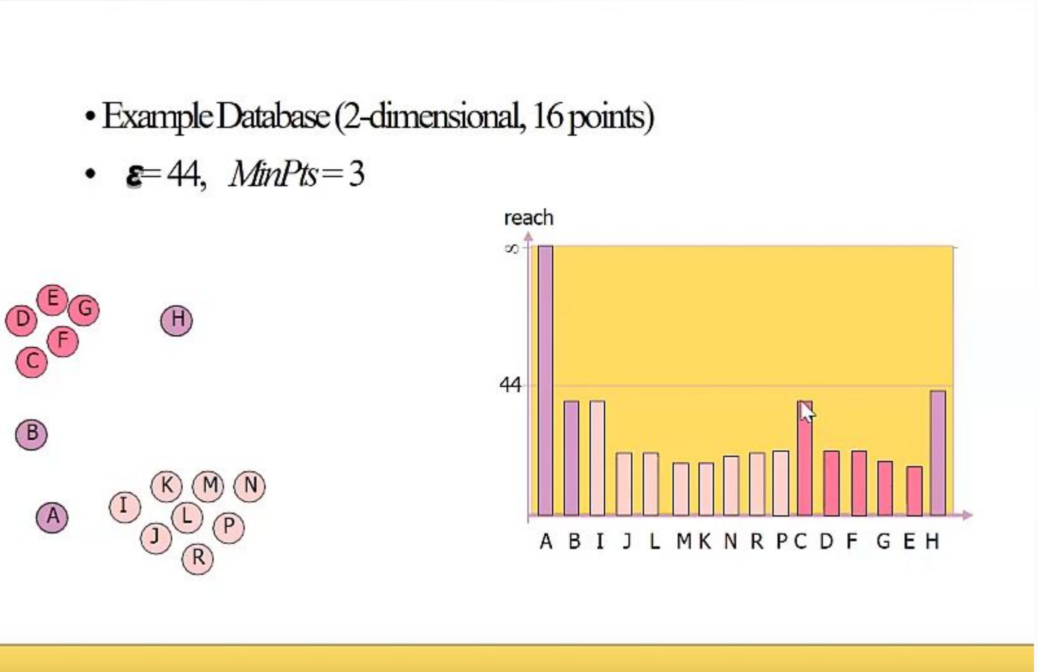


- The valleys represent the clusters.

Min neighbours:3

OPTICS

Explanation from:
https://www.youtube.com/watch?v=CV0mWaHOTA8&t=133s



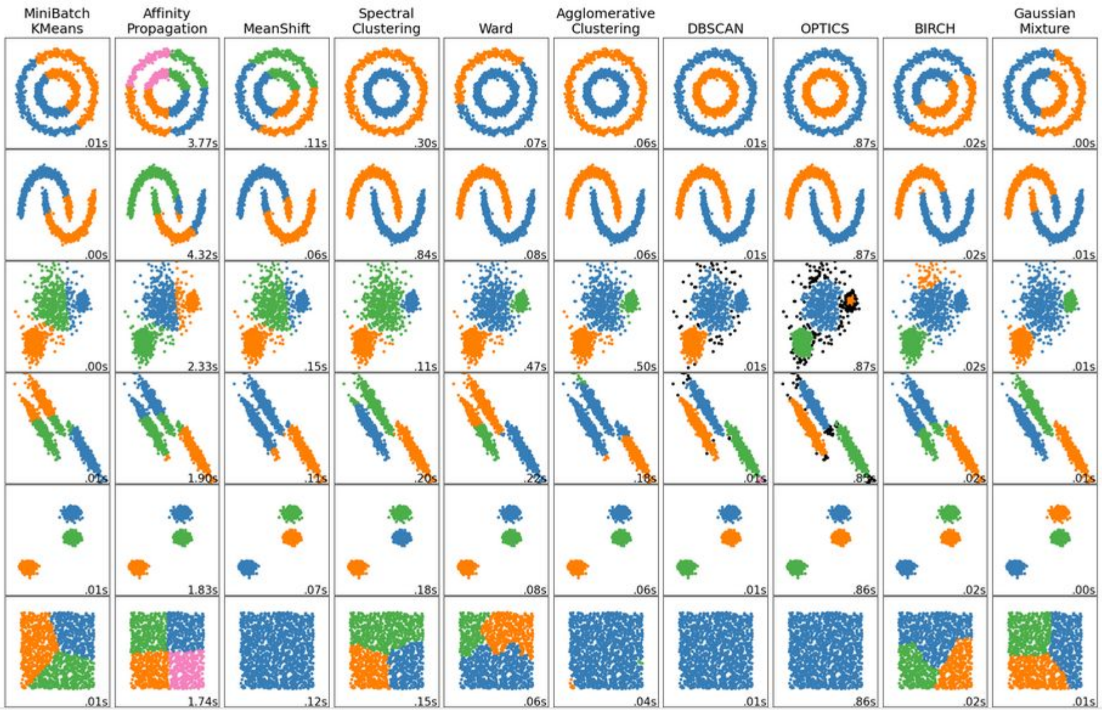
- The valleys represent the clusters.
- Parameter xi is parameter that is applied on the reachability plot in order to extract the clusters.

Min neighbours:2

Clusters

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

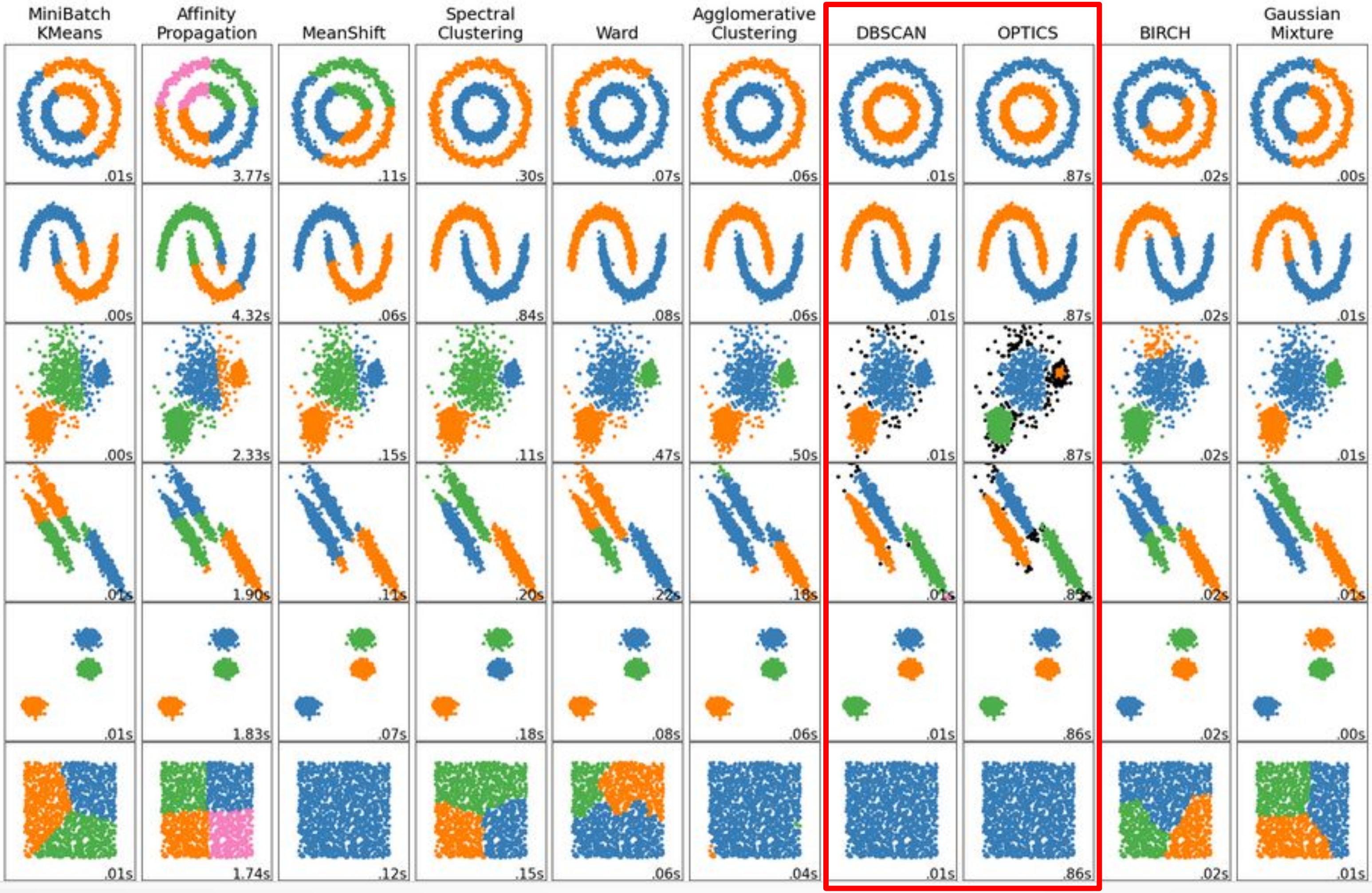
Image from[12,13]



- 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

12) 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.
13)https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py

Image from[12,13]

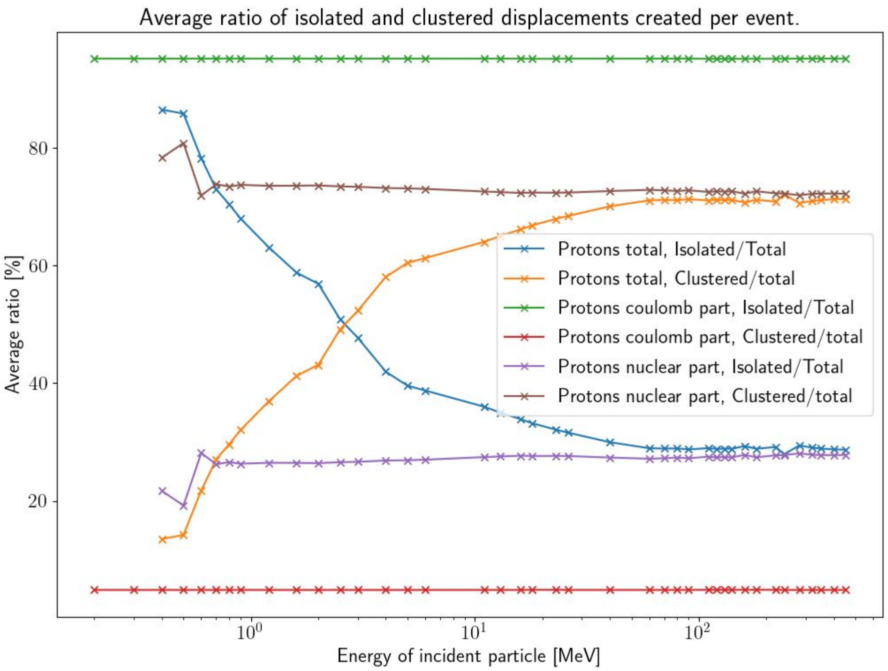


OPTICS performs better then DBSCAN for clusters with **varying densities**[14].

12) 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.
13)https://scikit-learn.org/stable/auto_examples/cluster/plot_cluster_comparison.html#sphx-glr-auto-examples-cluster-plot-cluster-comparison-py
14)https://scikit-learn.org/stable/modules/clustering.html#optics

RESULTS: protons (backup)

Results for n=9, xi =0.05

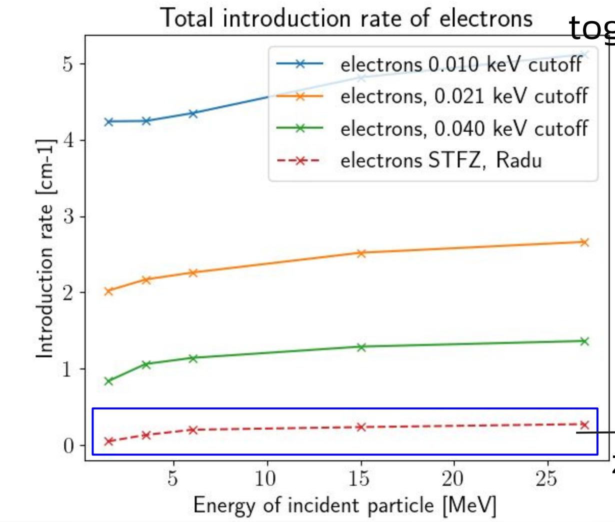


- For E> 100 MeV stable ratio of point-like and cluster like displacements for protons.
- For the protons it takes a longer time to reach the stable ratio of the cluster and point defects, because of the decreasing ratio of the cross section for Coulomb scattering / Nuclear (elastic+inelastic scattering)

Electron induced damage

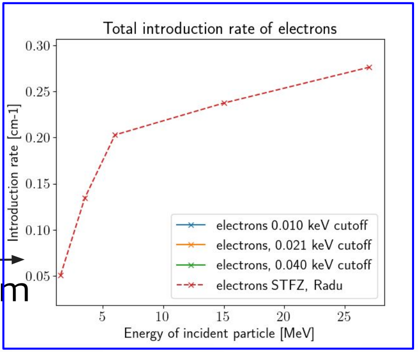
Work in-progress

VOi, V3 and V2 together

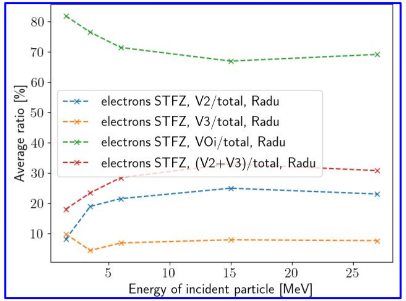


zoom

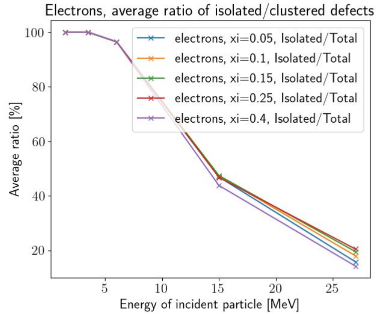
Total introduction rate from Radu is approx 10 ~ lower.

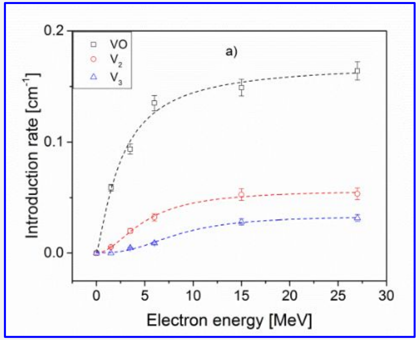


Ratios from Radu



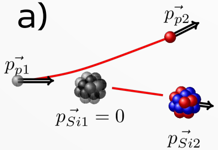
Ratios clustered/total from Geant4



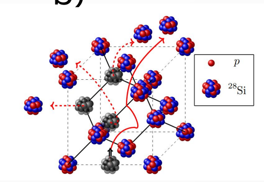


R. Radu: Bulk radiation damage in silicon:
from point defects to clusters

a)

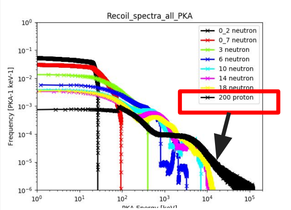


b)

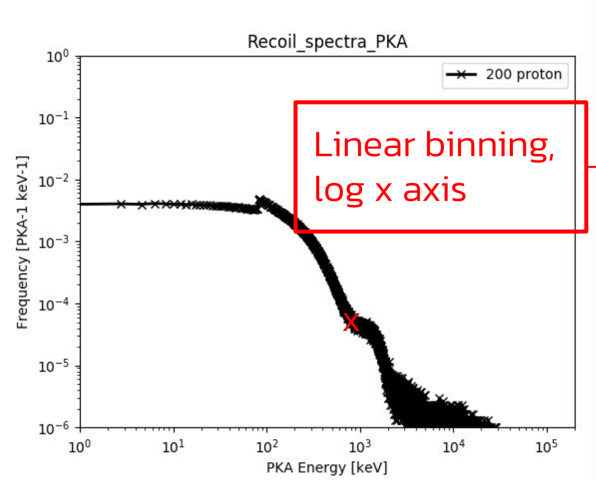


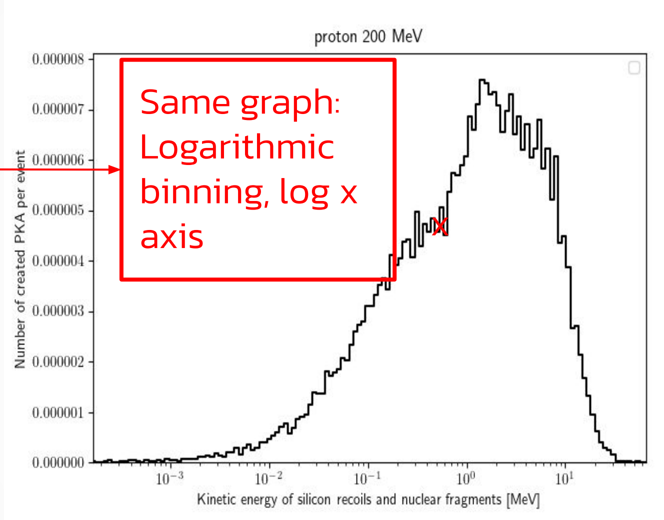
- The aim is to tune the parameters by using the measured values that we know.
- We would like to compare the total introduction rates and the rates between clustered and point defects.
- Tuning might depend on n, xi, cutoff limit.
- One of the options for the fine tuning would be to use a different constant for the processes that create only 1 PKA (a) and processes that create many SKA afterwards

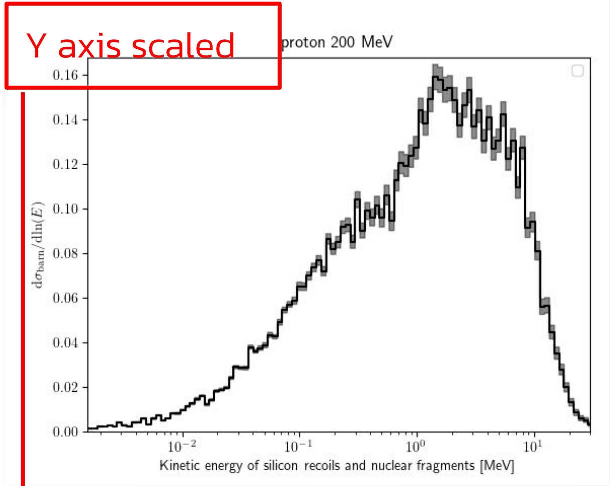
Keep only some of the plot



note: representing y axis as $\partial\sigma_{barn} / \partial \ln(E)$







1) PKA are summed and divided by the number of incident particles.

2) Logarithmic binning is used instead.

3) Each content in a bin is divided by the length of the bin. That makes the y-axis linear. Furthermore the y axis is scaled by:

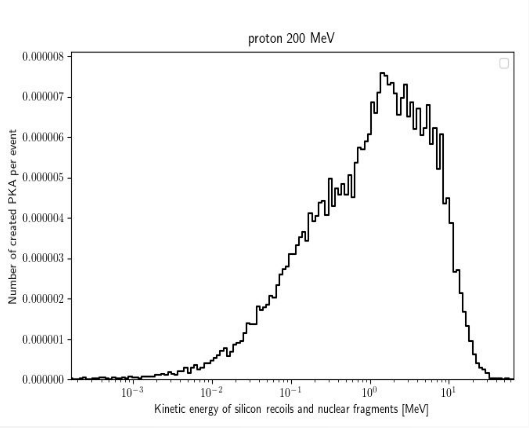
$$\frac{10^{24}}{N_{targ} d} \qquad d = 0.01\text{cm} \qquad N_{targ} = \frac{N_A \rho_{Si}}{m_{Si}}$$

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

Conversion from σ to probability:

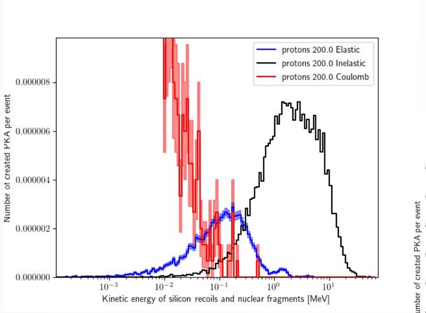
$$\frac{I_{scattered}}{I_{incident}} = \frac{N_A \rho_{Si} d}{m_{Si}} \sigma = 0.0005 \sigma_{barn}$$

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

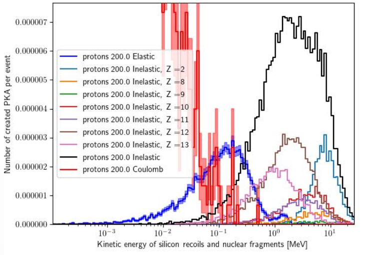


1) PKA are summed and divided by the number of incident particles. Logarithmic binning is used instead, that makes the y axis linear.

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 used[12].

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

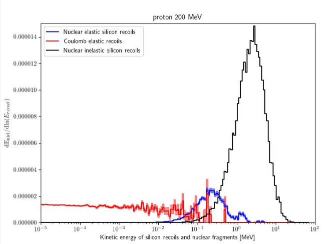
$$E_{\mathrm{de}} = \frac{E_{\mathrm{Si}}}{1 + k \times g(\epsilon)}, \quad (2)$$

with $k = 0.1462$, $\epsilon = 1.014 \times 10^{-2} \times Z_{\mathrm{Si}}^{-7/3} \times E_{\mathrm{Si}} = 2.147 \times 10^{-5} E_{\mathrm{Si}}$ and the universal function

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

5) For alphas[13], 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, https://doi.org/10.1109/TNS.2016.2574961.
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.