Simulating primary ionisation in Garfield++

New Horizons in TPCs, 5 October 2020

Outline

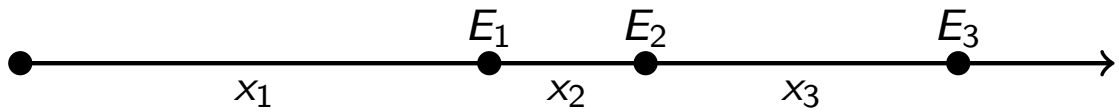
- Photoabsorption Ionisation (PAI) model, HEED.
- Primary electrons, DEGRADE.
- Heavy ions, SRIM.
- Opportunities for improvements and new developments.

For a Monte Carlo simulation of the energy loss along a charged-particle track we need the

- inverse mean free path between ionising collisions λ^{-1} (aka cluster density), and the
- probability distribution $f(E)$ for a particle to lose an amount of energy E per collision.

When then follow the charged particle from collision to collision,

- drawing a step length $x_i = -\lambda \ln r$ using a random number $r \in (0, 1]$, and
- sampling the energy loss E_i in each collision according to $f(E)$.



We can calculate λ^{-1} and $f(E)$ from the differential cross-section $\mathrm{d}\sigma/\mathrm{d}E$,

$$\lambda^{-1} = N\sigma = N \int \mathrm{d}E \frac{\mathrm{d}\sigma}{\mathrm{d}E}, \qquad f(E) = \frac{1}{\sigma} \frac{\mathrm{d}\sigma}{\mathrm{d}E}.$$

On the next couple of slides, we outline how to derive the expression for $\mathrm{d}\sigma/\mathrm{d}E$ used in the PAI model, starting from classical electrodynamics.

- Consider a point charge ze moving with constant velocity $\mathbf{v}$ through a medium.

$$\rho = ze\delta^3\left(\mathbf{r} - \mathbf{v}t\right), \qquad \mathbf{j} = \rho\mathbf{v}.$$

- The response of the medium is characterised by the dielectric function ε relating the displacement field $\mathbf{D}$ and the electric field $\mathbf{E}$,

$$\mathbf{D}\left(\mathbf{k},\omega\right) = \varepsilon\left(\mathbf{k},\omega\right)\mathbf{E}\left(\mathbf{k},\omega\right), \qquad \varepsilon\left(\mathbf{k},\omega\right) = \varepsilon_1\left(\mathbf{k},\omega\right) + \mathrm{i}\varepsilon_2\left(\mathbf{k},\omega\right).$$

- The electric field due to the polarization of the medium creates a force on the moving particle which slows it down. The average energy loss per unit distance is given by

$$\mathrm{d}E/\mathrm{d}x = ze\mathbf{E}\cdot\mathbf{v}.$$

- In the non-relativistic case (considering only the Coulomb potential), one obtains

$$\frac{\mathrm{d}E}{\mathrm{d}x} = -\frac{2z^2e^2}{\beta^2\pi}\int \mathrm{d}\omega \int \mathrm{d}k\,\frac{\omega}{kc^2}\,\mathrm{Im}\left(\frac{-1}{\varepsilon\left(k,\omega\right)}\right).$$

- Microscopically, the energy loss proceeds through discrete collisions with energy transfer $E = \hbar\omega$ and momentum transfer $q = \hbar k$,

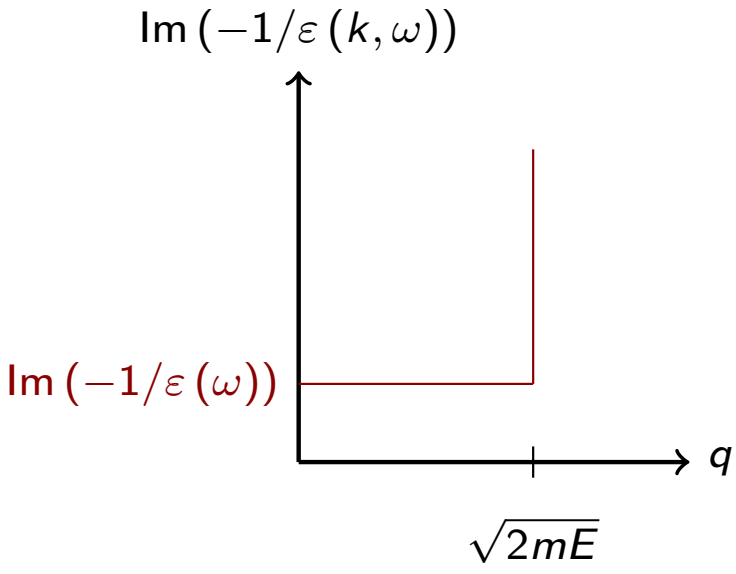
$$-\frac{\mathrm{d}E}{\mathrm{d}x} = N\int E\frac{\mathrm{d}\sigma}{\mathrm{d}E}\mathrm{d}E = N\int \mathrm{d}E\int \mathrm{d}q\,E\frac{\mathrm{d}^2\sigma}{\mathrm{d}E\mathrm{d}q}.$$

$$\rightarrow \qquad \frac{\mathrm{d}^2\sigma}{\mathrm{d}E\mathrm{d}q} = \frac{2z^2\alpha}{\beta^2\pi\hbar cN}\frac{1}{q}\,\mathrm{Im}\left(\frac{-1}{\varepsilon\left(k,\omega\right)}\right)$$

Calculating $\varepsilon(k,\omega)$ is, in general, quite complicated.

In the PAI model[1], the following simplification is made:

- at low momentum transfer, the optical dielectric function $\varepsilon(\omega)$ is used,
- a contribution from scattering off free electrons is added at $q^2 = 2mE$.



With this approximation,

- the integration over $q = \hbar k$ becomes straightforward,
- we only need optical data as input.

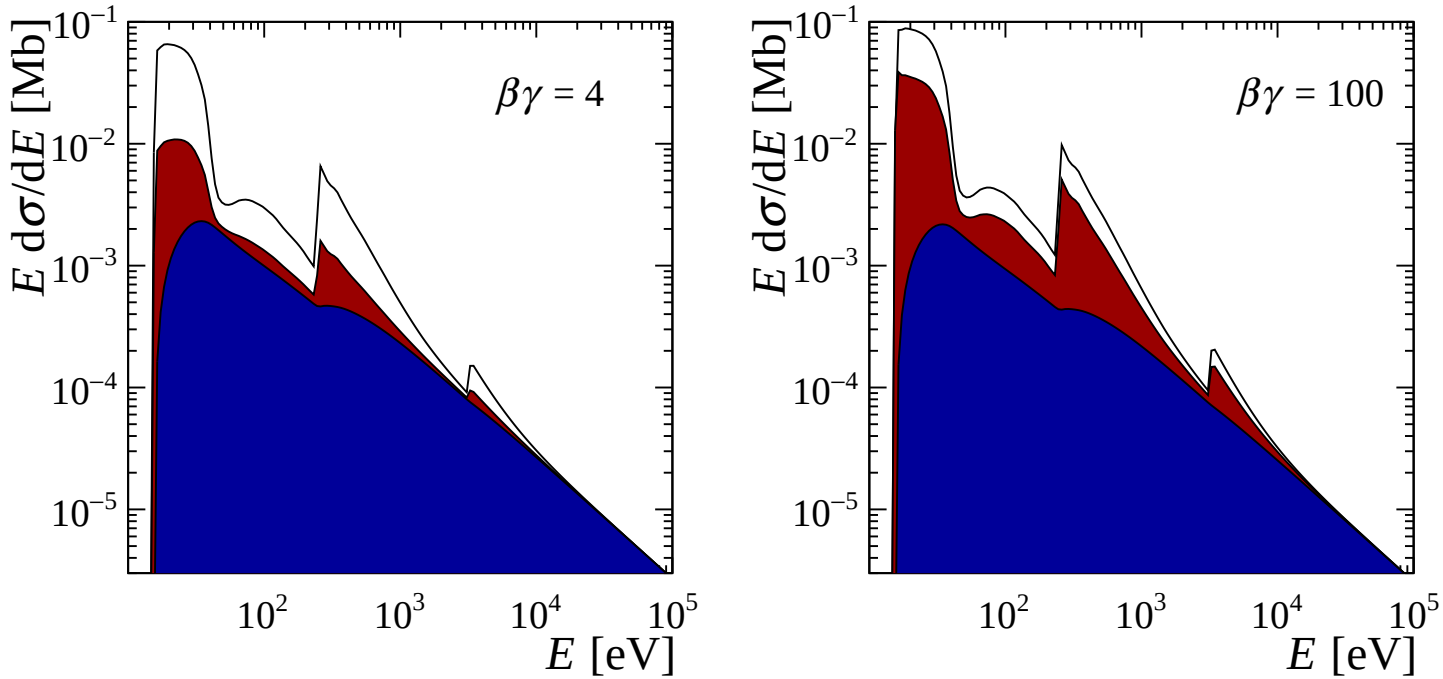
As a further approximation, we can calculate ε from the photoabsorption cross-section σ_γ,

$$\varepsilon_2(\omega) \sim \frac{N\hbar c}{E}\sigma_\gamma(\omega)$$

[1] W. W. M. Allison, J. H. Cobb, Annu. Rev. Nucl. Part. Sci. 30, 253 (1980)

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E} = \frac{z^2\alpha}{\beta^2\pi N\hbar c}\,\mathrm{Im}\left(\frac{-1}{\varepsilon(E)}\right)\ln\frac{2mc^2\beta^2}{E} + \frac{z^2\alpha}{\beta^2\pi N\hbar c}\,\frac{1}{E^2}\int_0^E E'\,\mathrm{Im}\left(\frac{-1}{\varepsilon(E')}\right)\mathrm{d}E'$$

$$+ \frac{z^2\alpha}{\beta^2\pi N\hbar c}\left[\mathrm{Im}\left(\frac{-1}{\varepsilon(E)}\right)\ln\frac{1}{|1-\beta^2\varepsilon(E)|} + \left(\beta^2 - \frac{\varepsilon_1(E)}{|\varepsilon(E)|^2}\right)\left(\frac{\pi}{2} - \arctan\frac{1-\beta^2\varepsilon_1(E)}{\beta^2\varepsilon_2(E)}\right)\right]$$



Differential cross-section for charged particles in argon, calculated using HEED.

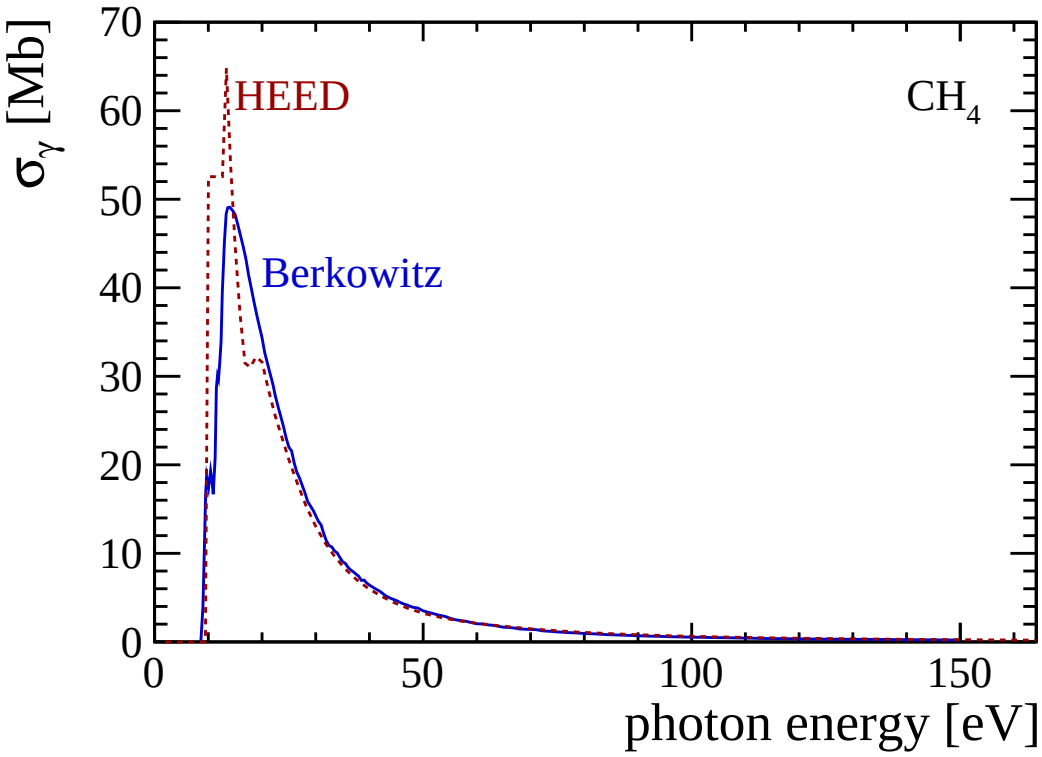
- The optical data used will influence the accuracy of the simulation results.
- The effect is most visible in the cluster density λ^{-1} (relevant for cluster counting), which is sensitive to the shape of σ_γ at low energies.
- HEED constructs the molecular photoabsorption cross-sections from the constituent atomic photoabsorption cross-sections.
- The agreement with data is quite good, but to improve on this approximation, one could try to use measured molecular photoabsorption cross-sections instead.
- One could, in theory, also try to improve the PAI model itself, and use calculated tables[2] of $\varepsilon(k, \omega)$ in the intermediate k range.

Gas	λ^{-1} [cm^{-1}]	
	Measurement[3]	HEED
Ne	10.8	10.5
Ar	23.0	25.4
Kr	31.5	31.0
Xe	43.2	42.1
CO_2	34.0	34.0
CF_4	50.9	51.8
CH_4	24.6	29.4
iC_4H_{10}	83.4	90.9

Cluster density for particles with $\beta\gamma = 3.5$, at $T = 20^\circ$ C and atmospheric pressure.

[2] D. Bote and F. Salvat, Phys. Rev. A 77, 042701 (2008)

[3] F. Rieke and W. Prepejchal, Phys. Rev. A 6, 1507 (1972)

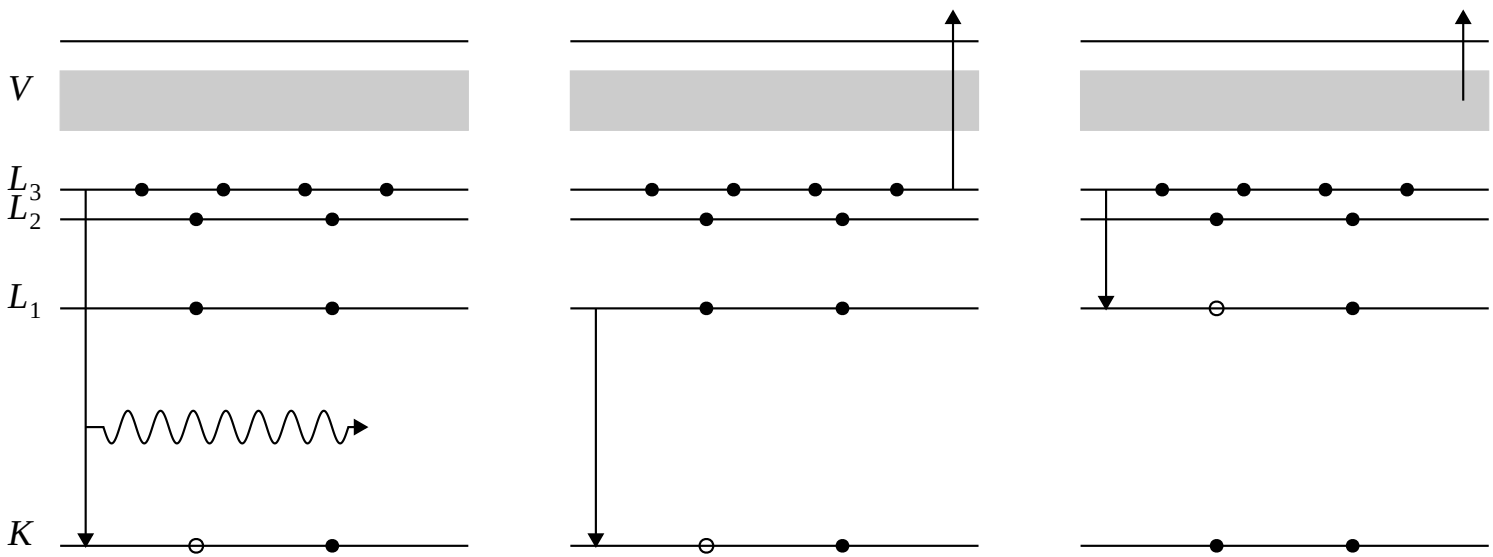


Photoabsorption cross-section for methane (approximation used in HEED, and data from NIFS-109).

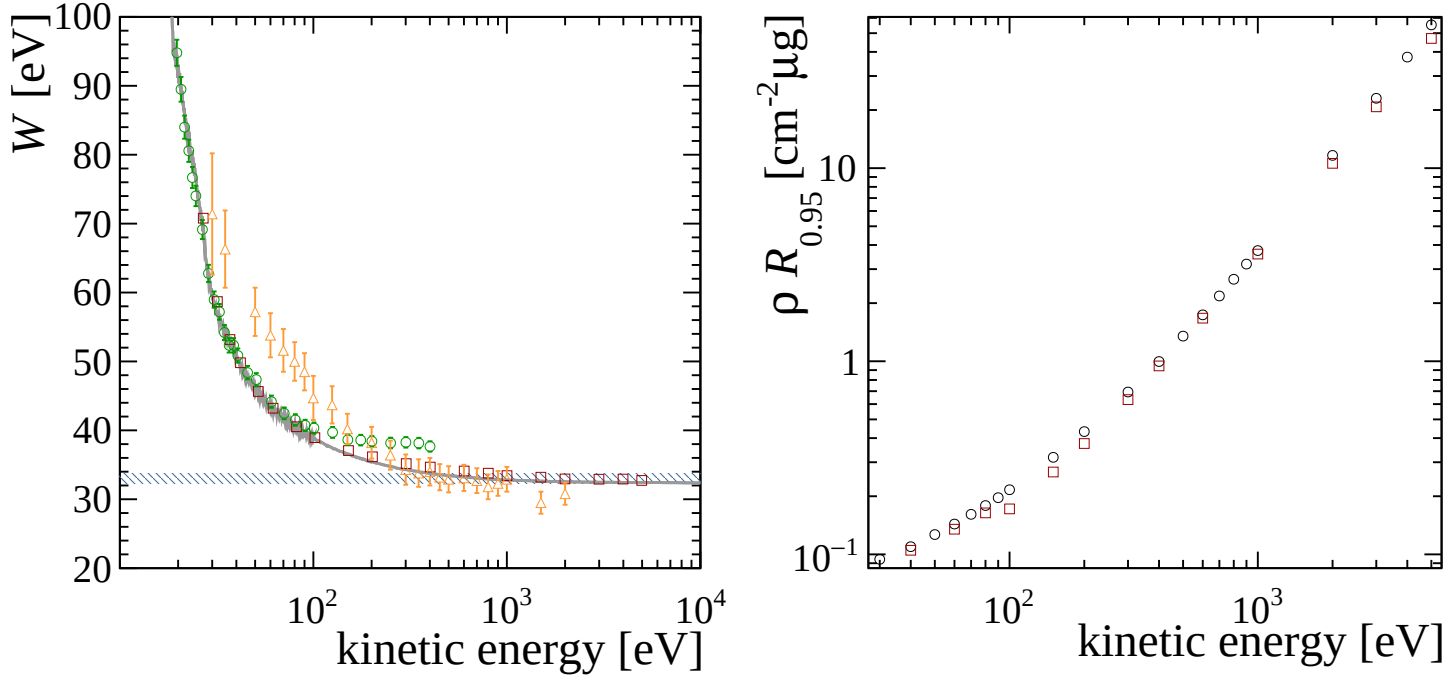
On a side note: photon transport

- Thanks to its cross-section database, we can also use HEED to simulate photoabsorption in a gas (or other media).
- We don't have dedicated tools in Garfield++ for other photon interactions (Compton scattering, pair-production) at the moment.

- Using the "plain" PAI model, we can simulate how much energy the primary particle lost in a collision, but not to which shell the energy was transferred.
- HEED splits $\mathrm{d}\sigma/\mathrm{d}E$ in contributions from each atomic shell, for details see Igor Smirnov's presentation at the last RD51 collaboration meeting or his paper.
- HEED also simulates the emission of fluorescence photons or Auger electrons following an energy transfer to an inner-shell electron.
- The simulation of the relaxation chain follows a simplified pattern.
- If applications require an accurate simulation of emission lines or Auger electron spectra, a more realistic set of transition probabilities would need to be implemented.



- The last element in the simulation chain is the transport of the (delta) electrons.
- HEED uses a phenomenological algorithm that reproduces statistically a given work function W and Fano factor F.
- Alternatively, one can take a microscopic approach and simulate the delta electrons using the cross-sections implemented in Magboltz.
- Recent versions have separate cross-sections for inner-shell ionisation and models for emission of Auger electrons and fluorescence.

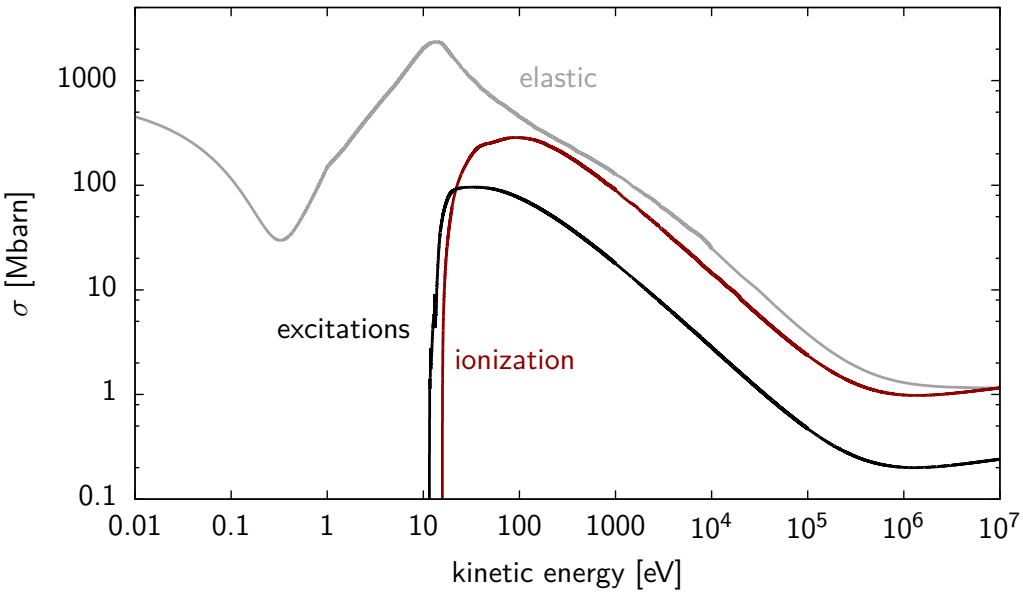


- Left: W value for electrons in CO_2 simulated using Magboltz (grey band) compared to experimental data.
- Right: electron range in methane (at atmospheric pressure) simulated using Magboltz (grey circles) compared to experimental data.

DEGRADE

- The techniques used in Magboltz for simulating electron transport can also be used for "primary" electrons (in the minimum-ionising energy range and beyond).
- Degrade is a "companion" program to Magboltz, by the same author (Steve Biagi).
- It is currently available[a] as a standalone (Fortran) program.
  Interface to Garfield++ to be written.
- In addition to electrons, Degrade can also be used for simulating X-rays.

[a] http://degrad.web.cern.ch/degrad/



Total cross-sections for electron scattering in argon, as implemented in Magboltz/Degrade.

$$\frac{\mathrm{d}\sigma}{\mathrm{d}E} \propto \frac{1}{E^2 + w^2}$$

Parameterization of the differential cross-section used for sampling the secondary electron energy in an ionising collision.

Limitations of the PAI model/HEED

- The PAI model loses validity when the velocity of the incident particle is no longer large compared to the velocities of the atomic electrons.
- To simulate slow particles (particles that are absorbed in the gas), we need other models.

SRIM

- Garfield(++) can import tables of stopping power, range, and straggling parameters as function of the ion energy calculated using the SRIM program.
- It will account for track-by-track fluctuations by sampling the energy loss from a Landau/Vavilov/Gaussian distribution (see the technical note by Rob Veenhof).
- An example is available on the website.
- Classic (Fortran) Garfield also has an interface[a] for importing individual events simulated using TRIM. If this is of interest, it can be ported to Garfield++.

[a] J. E. Butterworth and C. J. Barton, JINST 4 (2009)

Last not least. . .

- By interfacing Geant4 and Garfield++, a wide range of physics models becomes available[a].

[a] D. Pfeiffer *et al.*, NIM A 935 (2019)