Software tools for detector physics simulations

ECFA Symposium, 29 April 2021

Outline

- Recap of simulation tools (Garfield, Magboltz, Heed, ...).
- Challenges, open issues, opportunities for future developments.

Standard recipe

- Calculate the static electric field.
  - Analytically or using FEM (Ansys, Comsol, Elmer) or boundary-element (neBEM) field solvers.
- Simulate the number of electron-ion pairs produced by a charged particle track and their spatial distribution.
- Simulate the drift lines of the primary and secondary (avalanche) electrons.
- Simulate the ion drift lines.
- Calculate the current induced on a readout electrode using its static weighting field.
  - Optionally, add noise and convolute with the transfer function of the front-end electronics.

Primary ionisation

- Energy loss by relativistic charged particles is well described by the PAI model.
- HEED (I. Smirnov) implements an extended version of this model, simulating also atomic relaxation and delta electron transport, such that one obtains the coordinates of all ions and low-energy electrons produced along a track.
- If needed, some minor refinements could be envisaged, *e. g.*
  - using molecular instead of atomic photoabsorption cross-sections,
  - implementing a more detailed simulation of atomic relaxation.
- In case of projectiles for which the PAI model is not applicable, a possible solution is to interface GEANT4 and GARFIELD++, see *e. g.*
  - D. Pfeiffer *et al*, NIM A 935 (2019), 121,
  - I. Katsioulas *et al*, JINST 15 (2020), C06013.
- DEGRADE (S. Biagi) simulates ionisation by electrons, using the same set of cross-sections as MAGBOLTZ. Interface to GARFIELD++ to be developed.

Electron transport properties

- MAGBOLTZ (S. Biagi) calculates transport coefficients[a] using a Monte Carlo technique.
- Accuracy of the calculation depends on the quality of the electron-atom/molecule cross-sections used. MAGBOLTZ includes a library of carefully curated cross-sections for 55 commonly used gases.
- Continuous effort to improve the quality of the cross-section data (collaboration with LXCAT) and add new gases (including alternatives to greenhouse gases).
- ⚠ Relies on work by few experts.
- Recent efforts to refactor the code, *e. g.* PyBoltz.

[a] drift velocity, diffusion coefficients, Townsend coefficient, attachment coefficient.

Simulating electron avalanches

- Microscopic[a] tracking (Monte Carlo simulation based on electron-atom/molecule cross-sections à la MAGBOLTZ) has become standard for MPGDs.
- Easy to use and important for simulating stochastic effects, but can become slow when dealing with high gain and/or large distances, in particular for complex fields.
- Could profit from code optimisation to better exploit modern CPUs (or GPUs), and clever ideas for transitioning to a "mesoscopic" technique at large avalanche sizes.
- We usually assume that the electrons move in a static field, independently from each other. If that assumption is not valid, things become complicated.
- In theory, space charge could be taken into account by iterative field calculations. In some cases one can use shortcuts like limiting the avalanche growth to a certain size.
- Dealing with space charge is much more straightforward in hydrodynamic simulations.
  - F. Resnati, RD51 Open Lectures, December 2017
  - P. Fonte, RD51 Collaboration Meeting, June 2018
- This approach has been used successfully for simulating streamers and discharges.
- Another example of dynamic effects: charging up in a (TH)GEM.
  - P. Correia *et al*, JINST 9 (2014), P07025
  - P. Correia *et al*, JINST 13 (2018), P01015
  - Possible, but time consuming.

[a] As opposed to calculating the average drift path based on macroscopic transport coefficients.

Excitation transfer

- MAGBOLTZ includes detailed cross-sections for noble gas excited states.
  Deexcitation can contribute significantly to the gain in mixtures (Penning effect).
- Ongoing programme to determine effective Penning transfer probabilities from fits to measured gain curves → growing encyclopedia of transfer probabilities.
  - Ö. Şahin, New Horizons in TPCs, October 2020
- At the moment, one still needs to specify these parameters "by hand" in GARFIELD++ simulations (by default, Penning transfer is not taken into account).
- In principle, Penning transfer could also be simulated microscopically. This requires a wealth of input data, however:
  - radiative transition rates, lineshapes, photoabsorption cross-sections and ionization yields,
  - rate constants and ionization yields for collisional quenching, ...
- These sets of data are also needed for a microscopic modelling of electroluminescence (*e. g.* in optical TPCs).
  - C. Azevedo *et al*, NIM A 877 (2018), 157
  - D. González-Díaz, New Horizons in TPCs, October 2020
- A lot of work ahead!

Ion transport

- Ion drift lines are simulated macroscopically, with a drift velocity $v_D = KE$ calculated from literature values for the (reduced) mobility $K_{(0)}$ – if available.
  - One usually uses a single set of mobilities (corresponding to the ion species assumed to be "dominant") for all ions in the mixture.
- Reality is complicated: charge transfer, formation of clusters, ...
  - R. Veenhof, RD51 Lectures, June 2020
  - A. Cortez, New Horizons in TPC, October 2020
- A lot of work ahead!
- Should also add support for negative ions.
- Is there a need for simulating electron-ion recombination?

Signals

- For calculating the induced signal in geometries including elements with finite conductivity, we need an extension of the Ramo-Shockley theorem.
  - W. Riegler, NIM A 535 (2004), 287
  - W. Riegler, CERN Academic Training, December 2019
- The time-dependent weighting potential used in this formalism can be calculated analytically (for simple geometries) or using a FEM solver (Comsol).
  - D. Janssens, RD51 Collaboration Meeting, February 2021
- Next steps: apply the method to realistic detectors (*e. g.* resistive MPGDs).
- Formalism also applicable to transmission lines.
  - W. Riegler, P. Windischhofer, NIM A 980 (2020), 164471

Conclusion

- Detailed simulations are widely used tools for understanding and optimising the performance of gas-based particle detectors.
- Having a common platform, embedded in an R&D collaboration, is a key strength.
  - Long-term support. Close link to experimental activities.
- Ongoing work to address challenges in many interesting areas, including modeling of electron avalanches, deexcitation, ion transport, resistive layers, (dynamic) field calculations, *etc.*
- Interesting field of work combining software development, numerical methods, physics.