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**BACHELOR THESIS**

Tomáš Čelko

**Support for annotating and classifying particles detected by TimePix3**

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Title: **Support for annotating and classifying particles detected by TimePix3**

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# Introduction / Preface

In nuclear physics, there have been many efforts to visualize and detect elementary particles. For this purpose, various detectors were invented. Several such detectors are now members of the so-called Medipix detector family. The most recent member of the family is called the TimePix3 detector. In terms of elementary particle detection, TimePix3 achieves state-of-art performance. During a specified timeframe, the detector captures a set of particle trajectories. However, in some cases, a single particle emits the secondary particles that can interact. Instead of detecting the particles one by one, we analyze groups of such particles – so-called clusters.

So far, there have not been many publications dealing with the processing, filtering, visualization, or classification of these clusters. In the filtering task, one needs to make sure the algorithm is fast because the size of the cluster dataset captured by TimePix3 detector can reach gigabytes of data over a short timeframe. The classification process can be challenging because the trajectory of the cluster depends on the angle at which the particle enters the field of the detector. Furthermore, the distribution of various types of clusters in the standard observation is usually very uneven. For instance, most of the data received from detectors like ATLAS [link] contains only simple traces consisting of a few pixels and does not provide much information for the analysis. This fact causes problems for many machine-learning-based approaches because the datasets of the rare and more complicated clusters often have a minimal size.

**Goals of the thesis**

Our main goal is to create a set of processing tools that would enable physicists to analyze the clusters and their properties. The input will be a collection of cluster from the Clusterer application []. Firstly we need to provide support for filtering the clusters based on their attributes. Secondly, we visualize them individually so that the users can see the cluster as a 2D and 3D image. Because the number of clusters in some datasets can be overwhelming, another goal is to make a tool, which could calculate the properties for the whole collection of clusters. The calculated properties of the clusters should enable to design a neural network-based classifier capable of classifying various clusters, which is our final goal. Eventually, the developed classifier could also detect extraordinary clusters, displaying exotic or even unseen particles.

**Thesis layout**

**Related work**

* Detecting elementary particles with Timepix3 detector [4]

# Analysis

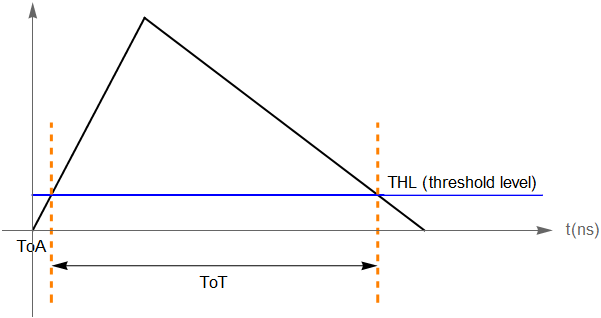
In this chapter we discuss the detection of elementary particles with hybrid pixel detectors, as well as the tools and methods suitable for the analysis of the detector output. Firstly, we introduce the Medipix detector family, then we present the format of the data from the Timepix3 detector. We also introduce new types of neighboring relation for the pixels. Then we move to the visualization of the Timepix3 data and last but not least we discuss the classification methods for the groups of elementary particles called clusters.

## The Medipix family and the TimePix3 detector

It was the 1990's when some of the researchers from CERN came with an idea to transfer the devices, primarily developed for experiments in Large Hadron Collider(LHC) beyond particle physics. The first collaboration with such a goal started under the name Medipix1. It was the collaboration of the University of Freiburg, University of Glasgow, and Napoli and Pisa Universities together with CERN. So far, there have been four Medipix collaborations, each with its own specific goals. The chips developed in these collaborations are known as the members of the Medipix detector family.

The first member of the family was the Medipix1 chip (1997), consisting of 64 x 64 pixels acting similarly to an digital camera – counting the hits of elementary particles while the shutter is open. A few years later, the Medipix2 chip was developed, leading to the first Timepix chip (2006) being invented. This was the first chip that can be programmed to record one of the following properties:

* **Particle hit count:**  The number of hits detected by the pixel in one tick of the internal clock. (similar to Medipix1)
* **Time over the threshold:** Each pixel is assigned an energy threshold level(THL). When a charged particle approaches the pixel, the energy captured by the pixel rises. The time interval while the energy remains above the threshold we call the time over the threshold (ToT). This attribute is often measured as the number of ticks of a detector clock.
* **Time of the arrival:** – The absolute time since the start of measurement until the energy threshold level is reached we call the time of arrival (ToA).



In 2013 the new TimePix3 chip was introduced to the family. "Timepix3 is a general-purpose integrated circuit suitable for readout of both semiconductor detectors and gas-filled detectors. Compared to its predecessor Timepix the circuit has more functionality, better time resolution, and more advanced architecture for continuous sparse data readout with zero-suppression." [1] Zero-suppression means that there is no data output from the detector unless nonzero energy input is captured. This allows better efficiency in data collecting and storage but also in data analysis. The device utilizes a 256x256 pixel matrix where the size of each pixel is 55μm, achieving a time resolution of 1.56ns. The TimePix3 chip is nowadays used in the CERN LHC to detect sets of elementary particles, so-called clusters.

## Input format and calibration

Because the output of the TimePix3 chip over some timeframe can contain multiple clusters, we use the Clusterer application [4] to process the raw input from the detector and separate the clusters from each other. This means that instead of processing the data in the raw format, we use the data in the MM (clustered) format. The MM data format consists of three text files – ini, cl, and px file.

* Ini file contains the name of the measurement and the names of the cl and px files associated with the given measurement. By default, this file expects to find the cl and px file in the same directory where the ini file is located
* Cl file consists of the primary data about the cluster collection, where each line represents a single cluster. A line contains the first time of arrival of the cluster in ns (since the start of the measurement). This is followed by the size of a cluster and the number of the line in the px file (and the number of the byte) where the cluster starts.
* Px file includes data about each pixel in the cluster, namely and coordinates of the pixel, the time of arrival in ns, and the energy in keV.

|  |  |  |
| --- | --- | --- |
| **FILE** | **FORMAT** | **EXAMPLE** |
| ini | [Measurement (or any string ending with a newline char)] PxFile=[Relative path from the parent direcotry of .ini to px file]  ClFile=[Relative path from the parent direcotry of .ini to cl file] | Measurement 123 PxFile= Clusters\_px.txt ClFile= Clusters\_cl.txt |
| cl | [First ToA (float)] [Pixel Hit Count ( integer 0-232)] [LineOfStart in px file ( integer 0-232)] [Byte of start in px file (integer 0-232)] | 12345.647 100 5 30 |
| px | [x coordinate of the pixel ( integer 0-255)] [y coordinate of the pixel (integer 0-255)] [ToA (decimal)] [Energy (decimal)] | 123 128 15540 14.235 |

Table 1.1 Input MM file format

There are two kinds of MM formats, which only differ in the px file:

* ***Calibrated*** data have the structure as displayed in the chart []
* ***Non-calibrated*** data are very similar to the calibrated ones, but instead of the energy attribute in .px file, they use the attribute

To determine whether a file is calibrated or non-calibrated, we can open the px file and look for the last column. If the decimal part of the values is zero in every pixel, we know we are dealing with non-calibrated data because the is measured as a number of ticks of the detector, which is an integral value. However, if the values have a non-trivial decimal part that indicates the data is already calibrated.

The calibration is the process of replacing the attribute with the corresponding energy. The energy deposited in the pixel is a function of the but also four other parameters of a pixel, denoted by the letters , , , and . These parameters are set during the measurement and are usually stored in separate text files as a 256x256 matrix of decimal numbers. It holds:

In the equation, *E* represents the energy deposited in the pixel, with *a*, *b*, *c,* and *t* being the calibration parameters.

## A little about neighboring

Neighboring of the pixels is an essential term when it comes to 2D image analysis. In general, two pixels are called neighbors if there is a relatively small distance between them. To be more specific, there are two known kinds of neighbors:

|  |  |  |
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|  |  |  |

* ***8-neighbors of a pixel p***

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* ***4-neighbors of a pixel p***

And for future use, we will also recognize another kind of neighbors:

* ***Y-neighbors of a pixel p***

This kind of neighbors has two main variants:

Variant AVariant B

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For each variant, we also consider their symmetric alternatives to belong to the same variant.

## Calculating the features

A cluster can be defined as a set of pixels, each containing information about its and coordinates, and energy. Apart from these explicit features, we also analyze the implicit features of the cluster like pixel count and the cluster’s total energy. This is the critical point of all our following work and also the main topic of this subchapter. We briefly discuss the features and the information they indicate about the cluster. The properties we can calculate range from straightforward to more sophisticated. The most important features are the following:

* ***Total, average and maximum energy, the standard deviation of energy,*** and ***low energy pixels count***provide information about the energy distribution of pixels in a cluster. The total energy of a cluster is defined as a sum of the energies of each pixel in the cluster. A pixel is considered to have low energy if its energy is less than 10keV.
* ***Pixel count*** attribute reflects the size of a cluster
* ***Width(diameter)*** and ***convexity*** attributes are both based on the convex hull of a cluster. Let denote the vertices of the convex hull of a cluster. Then the convexity is defined as follows:

The convexity of a cluster provides us the information about its shape because the more complicated clusters usually tend to have a concave shape. In contrast, the simple ones are often more convex. Width, also commonly know as the diameter, is defined as where *d* represents the distance between given vertices. For the function *d,* we chose to use the Euclidian distance in a plane: where is a pixel with the coordinates and .

* ***The standard deviation of the ToA*** captures the information about the timespan of a cluster. Another option would be to use the difference of the . This, however, has a disadvantage because in a cluster, there are often a few pixels that show extreme values of ToA. The standard deviation is considered to be "more resistant" to these outliers pixels and provides a reasonable estimate of the timespan of the cluster.
* ***Vertex count, Crosspoint count,*** and ***Branch Count*** reflect the possible number of particles in a cluster and the shapes of the trajectories in the cluster. A pixel is considered to be a vertex if it only has one neighboring pixel. Crosspoints are the pixels where the trajectories of different particles meet. These pixels we find as the ones with nonzero energy and with three or more 4-neighbors or 3 Y-neighbours with nonzero energy (both variants of Y-neighbors are possible). Crosspoints of a set are denoted by , and are displayed on the image (pink color)[]

******

Because we do the branch analysis iteratively we define the term branch found at the k-th iteration instead of a simple branch. A branch found at the *k*th iteration is a set of pixels defined as follows: Let *P* denote a set of pixels in a cluster *C*. Let denote a graph such that there exists a bijection *b* between *P* and *V*. Furthermore, for each pair of 8 - neighboring pixels in the cluster there is a corresponding edge in E*.* Then we say P is a branch found at the k-th iteration if and only if its corresponding graph G is a path, P has the maximal possible size, and at least one of the following conditions holds:

1. (base step of the definition), or
2. none of the pixels in P are part of any of the previousbranches in (inductive step of the definition)

## Cluster visualization

The clusters we obtain from the Clusterer [] can be represented as a set of pixels, each with its own value of and energy. These pixels can then be visualized on a 256x256 bitmap, where a pixel is assigned a color according to the value of the pixels attribute. In this subchapter we introduce some methods for further cluster analysis based on its 2D image. These methods include skeletonization, z-coordinate calculation, finding the center of a cluster and branch analysis.

*Skeletonization*

Skeletonization of a binary image is defined as the thinning process that outputs a simpler version of the original image, the so-called skeleton. An important requirement for skeletonization is to have the image in binary format – each pixel is either white or black. Because the image of a cluster is not binary, we assign the value 1 to each pixel with nonzero energy and a value 0 to a pixel with zero energy. The skeleton should preserve the original shape of an image. In fact, the definition of skeletonization is not exact, which means various approaches can be used, each possibly outputting a unique skeleton.



For this purpose, we decided to modify Zhan-Shuen's algorithm for thinning binary digital patterns [6] in the following way:

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|  |  |  |  |
| 1 |  |  | |
| 2. |  |  | |
| 3 |  |  | |
| 4. |  |  | |
| 5. | If condition(S,p) and p.energy<t |  | |
| 6. |  |  | |
| 7. |  |  | |
| 8. |  |  | |
| 9. |  |  | |
| 10. |  |  | |
| 11. |  |  | |
| 12. |  |  | |
| 13. |  |  | |

Algorithm 1.1 Skeletonization of a cluster

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|  | as displayed in the figure [] |
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Figure 1.1 Example of pixel p with on indices (0,1), (3,4), (5,6)

The whole skeletonization process consists of using the twice. First time with value set to 10 keV and then we repeat the process with set to infinity. As a result, the first iteration aims to remove the halo effect of the low energy pixels while still preserving the shape. The second iteration with behaves the same as the original version of Zhan-Shuen's algorithm. A different approach would be to filter the low-energy pixels right away, but that does not guarantee that the cluster remains connected, which is a problem for future branch analysis. Because the thinning process returns non-trivial data for bigger clusters, we optimized the algorithm for those (~70-1000 pixels).

*3D reconstruction*

Because the Timpix3 detector is capable of capturing the particle energy, we are able to reconstruct its trajectory in 2D. However, Timepix3 also stores data about the time of arrival which can be used to estimate the z-coordinate of the particle. To provide the user with a 3D trajectory image, we need to calculate the z-coordinate. The z coordinate is a function of the relative time of arrival , where  is the difference between the arrival time of the particular pixel and the minimum time of arrival in the entire cluster. It holds:

[2]

Parameters used are the following:

*  - depletion voltage that is the minimum voltage at which the bulk of the sensor is fully depleted
* - bias voltage, which is the amount of voltage that a detector needs in order order to function [13]
*  - the electrical mobility of a hole
*  - thickness of the sensor

All parameters are specified at the beginning of the measurement and remain constant for the whole duration of the measurement.

*Center Finder*

When analyzing the shape of a cluster, it could be useful to know where the center of the event is. The center is usually the point with high energy located at the intersection of the visible trajectories (if there are any). If we manage to find this point correctly, we could then start analyzing each trajectory starting from the core pixel of a cluster event. However, this task proved quite challenging, especially for the complicated clusters, because there can be multiple points with the high energy level lying at the intersection of the trajectories. For this task, we proposed an algorithm based on the energy of the pixel and its surrounding pixels: Let C denote an arbitrary set of pixels and let  be the set of pixels surrounding the pixel (possibly where can be the Euclidian distance [] and ). Then, we define the weighted surrounding energy of a pixel with the weight as with being the energy of a neighboring pixel . For each pixel, the surrounding energy is used to calculate the center cost function.

Let represent the set of pixels of a cluster and let denote its skeletonized version. The center cost function is defined as follows:

In our algorithm, we set . Then the center pixel of a set of pixels is computed simply as the

*Branch Analyzer*

Before discussing the branch analysis, let us once again mention the definition from We say the branch  is a subbranch of the branch , if it starts in one of the crosspoints of branch b. To analyze the branches, we proposed the following algorithm:

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|  | | |
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| 2. |  |  |
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| 11. |  |  |
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| 13. |  |  |
| 14. |  |  |

Algorithm 1.2 Branch analysis

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| 0. |  |  |
| 1. |  |  |
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| 3. |  |  |
| 4. |  |  |
| 5. |  |  |
| 6. |  |  |
| 6. |  |  |
| 7. |  |  |
| 8. |  |  |

Algorithm 1.3 Get Branch function

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Figure 1.2 variables and function used in branch analysis algorithms

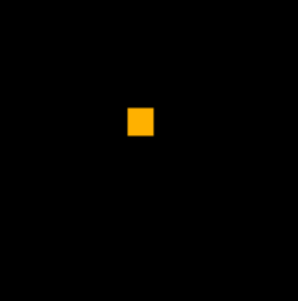
## Classification

After we are able to visualize clusters and analyze their properties, we can start focusing on subsequent classification. Firstly we briefly analyze the work done in terms of cluster classification. Then, we discuss the problems and the choice of the classifier model. Another topic we examine is generation of the training data.

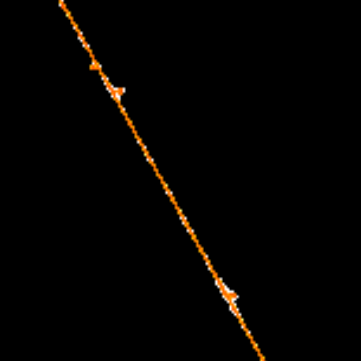
Classification of a cluster is a task where we are given a cluster and a set of possible classes. Based on the cluster, we should predict to which class the cluster belongs. Ideally, we also want to estimate how sure we are about our prediction and possibly return the result "unclassified" if we are not confident about the prediction.

So far, there have been a few attempts to classify clusters – one example being the work Detecting elementary particles with Timepix3 detector [4]. In this work, the clusters were divided into classes based primarily on their shape. The categories used in the thesis were the following:

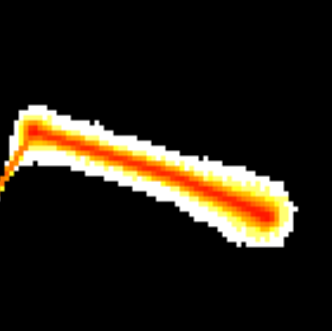
* Dot



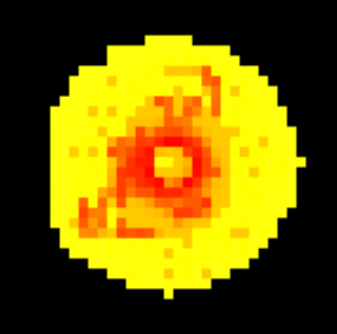
* Long gamma



* Heavy track



* Heavy blob



* Straight track
* Curly track



Even though this classification provides valuable information about the shape of a cluster, mapping these categories to the real particle examples is still non-trivial. For instance, one particle can have a dot shape when it traverses the detector perpendicularly. In contrast, if the same particle enters the detector's field in a direction parallel with the orientation of sensors, it could leave a straight or even a curly track, as shown in Figure 1.2.

|  |  |  |  |
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|  |  |  |  |

Figure 1.3 Possible 2D visualizations of the electron

The categories we decided to use for classification were based on the training data we were provided by Mr. [insert title] Declan Garvey, working at the Institute of Experimental and Applied Physics of the Czech technical university. The classes of the particles in the data were the following:

* Electron



Figure 1.4 Electron cluster image

* Muon

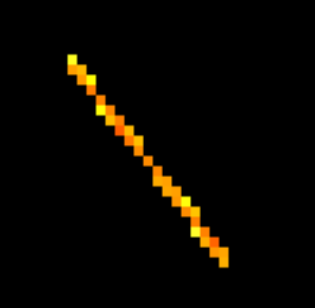


Figure 1.5 Muon cluster image

* Pion

Figure 1.6 Pion cluster image

* Proton



Figure 1.7 Proton cluster image

* He

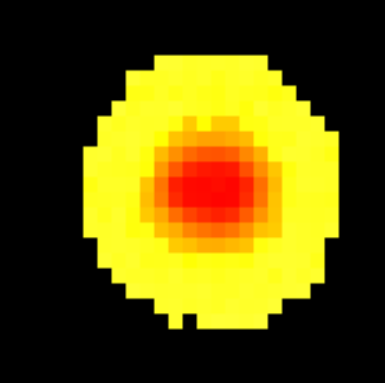


Figure 1.8 He cluster image

* Fe



Figure 1.9 Fe cluster image

* Fragmentation

Figure 1.10 Fragmentation cluster image

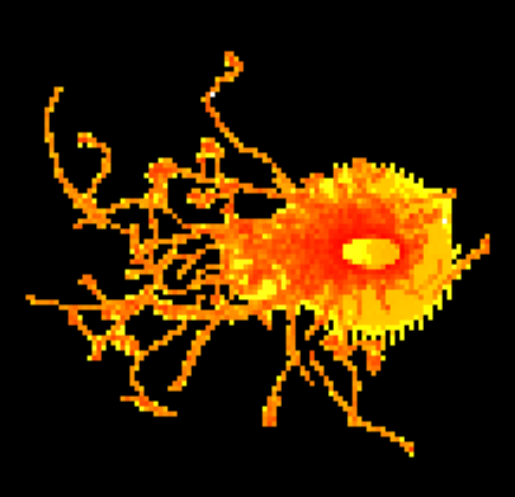
* Lead

Figure 1.11 Lead cluster image

Because it seemed to be very difficult to manually set the criteria for each class, we decided that a machine-learning-based approach could be a valid choice. We chose neural networks as these became very popular when it comes to solving complex problems, and in many tasks they achieve state-of-art performance. When fed with the data, the neural network model can learn from the data features until it reaches the maximum accuracy. There are many kinds of neural networks, but we narrowed the choice down to the two primary candidates – the convolutional neural network (CNN) and the multi-layered perceptron (MLP). The first candidate – the CNN – is widely used for the 2D image analysis, but it has a couple of drawbacks for our task. For instance, the cluster would have to be represented as a 2D image containing both the pixels with nonzero energy and also the ones carrying no energy. This means using CNN could be a little less efficient because CNN processes all of the given pixels (even though the zero energy pixels provide no information about the cluster). Considering the fact that we are able to calculate features and work with those instead of the whole set of pixels lead us to conclusion that we could use the feature-based MLP model.

*Training Data Generation*

Even though we had the data to train our model, the data were separated into files by particle type and angle of crossing the detector. This format can be great for viewing and browsing, but it is preferable to have one data source for training purposes. For that it is necessary to create an application that processes multiple files and generates a single training collection. When creating this application, we need to keep in mind that our dataset is likely have an uneven distribution of classes, so we need to add an option to spread the classes evenly.

# Goals of the thesis

Based on the obsevations from the Analysis chapter we formulated the main goals of the thesis:

* ***Cluster visualization*** – The commonly used MMFile format [Table 1.1] provides plenty of machine readable information about the clusters. However, for a physicist it can be difficult or even impossible to extract an intuitive overview about the cluster dataset from this format. This is why we decided to set the first goal to **provide an interactive cluster visualization tool, which would display various properties of a single cluster (like a 2D and 3D image of a cluster) while and also displaying a brief overview of the whole dataset**.
* ***Cluster filtering*** - Because we expect the input data to mostly contain regular and uninteresting clusters, we might need to select non-trivial clusters. In order to do that **we must create an application for filtering based on the attributes of a cluster. This application should focuse on the performance as we expect it to process a large amount of input data.**
* ***Classification*** – Because of the lack of tools for cluster classification, **we would like to create an interface which would provide a support for the classification of clusters by using the methods of machine-learning**. In order to create such classifier tool, we set two additional subgoals:
  + ***Data preparation*** – Before we start with the classification, **we must create an application which would prepare the training data for the subsequent classification.**
  + ***Classifier training*** – Because there can be different kinds of cluster dataset in the future we would like not to only create a single tool aimed for the classification of the specific clusters. Instead, **we want to create a parametrized interface for classifier training, which would enable the users to train and customize the classifier models based on their needs and the specific dataset.**

# Cluster Processor applications

## Specification

Based on the observations from the Analysis chapter, we decided to make a solution which consists of multiple applications – tools for viewing, analyzing and classifying the clusters. The reason why we split the solution into multiple applications is that this way it allows for a better extendability. When some developer comes with a better idea for classificator, he can still use the rest of our solution and adjust only the some part of the application. Another advantage of this approach is that each user can decide what functionality is required and download only the specific projects that cover the user’s requirement. All these tools are primarily made for physicists and could be divided into two categories:

* ***Interactive:*** 
  + ***ClusterViewer –*** an application for cluster visualization.The tool works interactively, which means after user input to view or analyze a cluster in responds immediately for the specific selected cluster. The application can display both 2D and 3D visualization of the cluster, and histograms of the cluster properties. Furthermore, the viewer can load a classifier classifier model of a user choice and use it on
* ***Non-interactive:***
  + ***ClusterFilterer –*** a project mostly for cluster filtering based on its features. User selects the desired interval for values of the attributes in UI and then the whole collection of clusters is processed at once.
  + ***DescriptionGenerator –*** a program which proceses multiple input files into one training dataset based on the preferred options selected in UI.
  + ***ClusterClassifier –*** a console application which takes trained classifier file and dataset of clusters in json format as an argument. The output of the application is classification of the whole dataset and splitting the data into multiple files based on the predicted class attribute.
  + ***ClusterClassifierUI –*** a user interface when it is possible to train your own classifier when provided classifier configuration parameters and the training data. Apart from training, user can also merge trained classifiers into multi-level classifiers.
  + ***ClusterTrainer –*** a console application which is capable of training a classifier after a configuration parameters and training data are provided.

## Cluster Viewer

In this subchapter, we will discuss all the features of the application for cluster visualization – ClusterViewer. This application contains tools to display and analyze the properties of a cluster. The features range from a simple 2D image to a 3D image and the analysis of the particle class.

*Input*

An input for the ClusterViewer application is a single ini file in the MM file format [Table 1.1]. This is selected via the user interface using either the dialog window or by typing the path to the file. Another option is to load a file in json file format which is an array of objects (clusters). This file format is an output of the DescriptionGenerator application and can be also an output of the ClassifierForClusters program. Each of the objects in the array must contain three specific keys in order to be successfully loaded. These are:

* ClFile – a relative path to the cluster cl file, starting from the directory of the application which created the file (it is recommended to have the ClusterViewer project in the same directory as the application which created the file)
* PxFile – a relative path to the cluster px file (similarily to ClFile)
* ClIndex – index of the given cluster in the cl file

Once the file is successfully loaded we can proceed to the other tools.

*2D view*

To get a better overview of the cluster dataset, we decided to create a 2D image of the clusters energy. The primary purpose of the image is to visualize the cluster as a bitmap, assigning colors based on the energy of the pixels. The viewer contains a 2D image that is represented as a 256x256 bitmap. In the cases where the same pixel is hit multiple times in a cluster, we decided to display the hit with the highest deposited energy. Because the low-energy pixels prevail in most clusters, we chose to map energies to color space logarithmically, which seemed to distinguish the energies without the need for a wide range of colors. For a more complicated cluster, this could also distinguish between halo pixels and the “real” particle trajectory.User can navigate through the currently loaded collection by clicking Previous and Next buttons, or by typing out the index and clicking the Find button. By using mouse wheel it is also possible to zoom in the cluster based on the position the cursor.

Figure 3.1 Cluster visualization indicating the halo pixels (yellow)

*Collection Histogram*

Another feature of the application is computing and presenting the Collection Histogram. That is the histogram of the currently loaded collection of clusters, representing the distribution of clusters with respect to PixelCount. The default option will display the histogram based on the cluster’s pixel count, but the program is easily extendable to accept any function of the cluster that returns a numeric value.

*Pixel Histogram*

Pixel Histogram works similarly to the Collection Histogram, except for the fact that it depicts the histogram of the pixels in the currently loaded cluster. The default displayed property of the pixel is its energy. This histogram could be helpful when deciding the class of a given cluster, because similar classes tend to have a similar energy distribution.



*3D Visualization*

Base on the ToA feature of the cluster, we calculated the coordinate according to the formula for the dependeny of the ToA from the coordinate of the pixel. This way we transformed two-dimensional points into three-dimensional, which we then showed visually as a 3D scatter plot. For a better viewing experience, we added an option to rotate the image around the x and y axes.



Figure 3.2 2D visualization of the cluster with linear trajectory

Figure 3.3 3D visualization of the cluster with linear trajectory



Figure 3.4 3D visualization of the cluster with multiple branches

Figure 3.5 2D visualization of the cluster with multiple branches

*Skeletonizer*

The differences in the output of the original algorithm and our modification can be seen in the figures []



Figure 3.6 Skeletonized cluster (modified Zhan Shuen's algorithm – [])

Figure 3.7 Skeletonized cluster (original Zhan Shuen's algorithm)

Figure 3.8 Orginal cluster

*Branch Finder*

One of the more sophisticated features of the ClusterViewer application is the BranchAnalyzer. Its main task is to analyze the given cluster and search for the possible trajectories of various particles in the cluster. These trajectories - branches are then distinguished by their colors. A branch is considered to be a main branch, if it starts in the center of a cluster. Each branch can also have its subbranches, which are denoted by the lighter version of their parent‘s branch color. For branch analysis we use the algorithm based on the breadth first search on the cluster‘s skeleton [Algorithm 1.1]. For the example of the branch analysis on a non-trivial cluster see figures [Figure 3.9] and [Figure 3.10].

**

Figure 3.9 Cluster after branch analysis, each branch with its distinct color (pink points are the cross points where the branches split)

Figure 3.10 Original cluster before branch analysis

## Cluster Filter

## Description Generator

The DescriptionGenerator is the application that was made to prepare the data (the features of a cluster) for the consequential training of the machine-learning based classificator model. The application requires the data to be in data in the MM (clustered) format [Table 1.1]. We also made the algorithm extendable to more features without requiring a lot of programming.

*Input selection*

 First, user selects and loads one or more ini files via the dialog window. All of the currently loaded files are displayed in the UI as shown in the [Figure 3.10]..

Figure 3.11 Loaded ini files into the DescriptionGenerator

All loaded ini files this way we call the class partitions or simply partitions. A partition can be assigned a class name, which is an editable field in the UI. These partitions are later grouped based on the class name to form the classes. The class names are compared as a strings one need to keep in mind the names are case sensitive. Apart from choosing input files, user must also select the name for the output file.

*Feature selection*

After the files are selected, user can choose which attributes will be calculated from the list. The algorithm is deigned to only calculate the features that are selected. Even though more features might provide more information about the cluster, adding features could also increase the time complexity of the algorithm and therefore the duration of the whole calculation.

For each cluster on the input, we calculate its features and store it into a single file in the Json file format. For bigger clusters the feature calculation complexities can be ordered into four categories according to the computational complexity:

Figure 3.12 Check boxes with cluster features

1. Expensive

* BranchCount
* Branches

1. Less expensive

* Width
* Convexity
* RelativeHaloSize

1. Inexpensive

* TotalEnergy, MaxEnergy, AverageEnergy
* VertextCount, CrosspointCount, RelLowEnergyPixels
* StdOfArrival, StdOfEnergy

1. Cheap

* Class, PxFile, ClFile
* PixelCount, ClIndex

Note - The complexity factor should be considered only for a large amount (gigabytes) of the input data.

*Distribution selection*

Before the processing we need to select the distribution of the input data in the output. For that we set the last parameters:

* ***Class distribution*** (even / proportional): When choosing even, each of the classes has a probability of to be the next class to process. If the option proportional is chosen, each class has a probability of being the next to process proportional to its size: where is the size of its cl file.
* ***Partition processing order*** (serial / parallel): Let represent the ordered partitons of a single class (based on the input order). After selecting serial, each class can proceed to the next partition only after the previous partition in the given class was processed (the whole partition, then the whole partition and so on). If the user chooses parallel option, and -th partition was processed in the previous iteration, then the next partition to process is the -th partition (when then reset to 0 to once again loop through the partitions).

Note: this order is only the order of partitions **inside** the class, keep in mind that each class is distributed by the previous parameter - Class distribution.

* ***Ending comdition*** (first class / last class / first partition): This condition sets when the processing should terminate. By choosing first class option, the algorithm ends when any of the classes is fully processed. When last class is selected, the program waits for all classes to be processed before terminating. If the user chooses the first partition option, then the program finishes as soon as any of the partitions of any class is depleted.
* ***Align class:*** When we set the optional parameter - align class - to the name of some of the classes in the loaded files, then the termination of the algorithm is only based on partitions of this align class and on the ending condition. All the other classes are meanwhile processed but with a single adjustion: When a partition of the non-align class is fully processed, it is not removed from the list, but it is only reset and will be processed once again. This means only the align class is being depleted while the others are repeatedly looping over their data.

Even though the first three parameters might actually seem useful at the first glance, one might wonder about the usefulness of the align class parameter. When we want to achieve even class distribution, we have two possible options:

* Downsampling[]
* Upsampling[]

One can notice that when choosing even class distribution (with ending condition on first class) and no align class, this is an example of downsampling. In constrast, if the align class is set, that can be considered an implementation of the upsampling. After all these necessary steps are completed, user can click the Process button which starts the processing and writing the output in a json text file, see the Figure 3.12.



Figure 3.13 An example of calculated features for a single cluster

## Classifier aplications

When we have the training data prepared by the Description Generator application, we can start focusing on developing the tools for cluster classification. For this purpose we designed three applications:

* ClassifierUI
* ClassifierTrainer
* ClassifierForClusters

Each of these applications uses a common type of neural network classifier model – a Multilayered perceptron (MLP). [] This type of model has many learning parameters which can be set that affects how quickly the model learns and how robust the model is.

*NN attributes and learning parameters*

|  |  |
| --- | --- |
| *name* | [any string] - used as a classifier **unique** identifier |
| *validAttributes* | [array of ClusterAttibute object] - sets the attributes of a cluster used during the learning process |
| *layerSizes* | [array of positive integers] - represents the sizes of the hidden layes |
| *activationFunction* | [“relu”, “sigmoid”] - sets one of the two currently supported activation functions |
| *learningAlgorithm* | [“leven-marq”, “backprop”] - chooses either the Backpropagation or Levenberg-Marqadt learning algorithm |
| *epochSize* | [positive integer] – the number of samples used in a single training epoch |
| *learningRate\** |  |
| *momentum\** |  |
| *evaluationMultiClasses\** | [array of pairs ([string], [array of strings])] – maps the prediction classes in the array to a new class name for the evaluation process (for example if our classifier predicts classes , and , we might want to analyze how well the classifier did at splitting class from the rest (using the accuracy)), so we map [(,[]),(, []) |
| *usedTrainDataSize\** | [a real number betwwen 0 and 1] – the proportion of data used for training (remaining data are used for testing) |
| *printInterval\** | [positive integer] – the frequnency of printing the training error of the neural network to the console |

Table 3.1 attributes and learning parameters of the classifier model stored in a config file (json),

*Classifier UI and Classifier Trainer*

The ClassifierUI is an application which aims to provide two main functionalities – classifier training and classifier merging. ClassifierTrainer is a console application which also provides classifier training (exactly the same as the ClassifierUI) but provides an option to run the learning process from the script without manual interaction. Because the training process is the same in the console application as it is in the UI, we will not discuss it separately.

***Classifier Training*** –Application trains a new classifier model based on the training data and the learning parameters data provided by the user. Some parameters like the minimal accuracy can be set directly via the UI but most of the learning parameters are set in a json config file, which must be loaded into the UI before learning starts. Optionally we can also load already trained classifier model and if done so, this model will be trained instead of creating a new MLP. By clicking Train Classifier we start the learning process. Then, the data is randomly split into training and test set according to the learning parameter (by default 90% training, 10% test). Information about error rate on the currently processed epoch are displayed into the console window. When the training is completed, the model is tested on the test data. To present the quality of the classifier we used the confusion matrix[] – a matrix where its element is the number of clusters that belong to the -th class and were labeled by the classifier as the -th class. So ideally we want to have the most cluster examples on the diagonal of the matrix. The result of the training process is what we call a simple classifier and it is stored in a two files with the suffixes .csf and .csf\_support. These two files should be in the same directory and preserve the same name at all times (they only differ in suffixes).

***Classifier merging*** – When we have a multiple simple classifiers we might have a need to concatenate their results in a single classifier with a tree-like structure. This can be especially useful, because as displayed in the [Figure 3.13], when we have classes with little training data (Classes A and B) we can create a root classifier trained on evenly distributed dataset by downsampling the larger classes (Class C and D). However, downsampling means not using some part of the training data which could negatively affect the accuracy of the model. Because it is possible to have more than one layer, we can train another classifier on the larger dataset (of Classes C and D) which enables us to:

* Use the most of the training data for learning
* Preserve the even distribution of classes among each level of the tree, which is preferred by many machine-learning based classifiers

Figure 3.14 Example of a multilayered classifier with two layers (Root classifier and Classifier 1)

Via the UI, it is possible to create a multi layered classifier with a maximum of 4 levels and on each level there can be a single classifier at most. This is because it can be quite complex to build any tree via the UI and also we expect this version to be sufficient for most cases. With a little programming user can build any classifier tree by simply connecting the nodes [].

To merge classifiers into a multi layered classifier user imports the trained model and if it is not the final layer, user also specifies the split class, which is the name of the class that will be further processed by the classifier on the next layer. This means if we input simle classifiers for merging, we should also input corresponding split classes. Then the name of the output is selected and when the merging is completed two output files are created - .csf and .csf\_support files.

*Classifier For Clusters*

The ClassifierForClusters is a console application such that when it is provided a trained classifier model and the cluster data in json format it can classify the given collection and provide an output based its parameters. There are three possible types of the output:

* ***Frequencies:*** The application prints the key value pairs of the name of the class and its frequency in the data
* ***Classes:*** The program outputs a single json file for each of the classes which contains the clusters that were predicted to belong to the particular class.
* ***Specials:*** When selected this option, the output of the program is similar to the Classes option but moreover it outputs a file where all the unclassified clusters that match a spefic criteria (potentially rare clusters) are stored. Changing this criteria is simple but requires a slight modification of the source code.

# Development documentation

In this chapter we will discuss the technical part of the solution ClusterProcessor. We will have a brief look into the implementation and the main objects and methods used in the solution. This section is primarily aimed for the developers who would like to find out how out solution works and those who plan to exted this solution in any way.

*Technology*

The framework we decided to use for the solution is .NET Framework and Windows Forms. The reason for that is simply because my primary programming language is C#, and I consider Windows Forms to be a reasonable choice for creating Graphical User Interface. However, WinForms does not support all features we reuired so we need the following external libraries:

* Chart Director [11] – a 3D graphical plotting library
* Newtonsoft.Net[] – a library (NuGet package) used for serialization and deserialization from the json file format
* Accord.Net[] – a machine-learning framework (NuGet package) we use for classification of the clusters

*Solution structure*

The whole solution represents a set of tools for cluster processing. The solution is structured into multiple separate projects mostly for two reasons:

1. User can choose which parts of the solution are desired and use only those.
2. This way the whole solution can be easily extended by modifying only one project a reusing the rest of the solution.

The projects in the solution can be divided into three layers according to their dependencies as shown in the [Figure 4.1]

Figure 4.1 Dependency structure of the ClusterProcessor solution

Cluster Viewer

Cluster Calculator

Classifier

Trainer

ClassifierForClusters

Descr Generator

Cluster Filter

ClassifierUI

Cluster Experiment

[should say how can the applications be extended, improved, how to create your own classifier]

## Main objects

C# as a programming language is well designed for object-oriented progamming and that is also the approach we chose to use. Each class represents an entity and these entities communicate with each other. This way we tried to design our program. In this section we would like to introduce a few main objects shared across the whole solution.

**PixelPoint** – an object for a single pixel, which stores it x and y coordinates, energy and the time of arrival

**Cluster** – a class which stores all of the necessary data for a single cluster, including an array of its pixels

**ClusterAttribute** – an enum attribute which can be computed and used as a training data for the classifier

**DefaultAttirbuteCalculator** – an object which can calculate the values of given cluster attributes when provided the cluster object

## Cluster Viewer

Even though the whole cluster viewer project consists mostly of the event handlers for the buttons of the application, but it uses some features from the ClusterCalculator which are worth noting from the software engineering perspective.

*Browsing Cluster Collection*

Browsing of the collection of clusters is done via the buttons. Without the chance of loading the data into operating memory, we need to search for a specific cluster sequentially each time we click previous. There is an option of creating a mapping table (index of a cluster, byte offset of a cluster) and then use .Seek() method (which might be faster, but could also consume a significant amount of memory). Another approach would be to use caching of the recently viewed clusters. We tested the browsing on the files with large cl files and did not notice any significant issue (browsing is done only on the cl file which is usually significantly smaller than the px file). Because of that we decided not to try optimizing browsing any further. Browsing is implemented by ClusterInfoCollection :IEnumerable.

*Skeletonization*

Skeletonization is the process of finding a skeleton of a binary image. For this purpose, we proposed an Algorithm 1.1. As the thinning process returns non-trivial data for bigger clusters, we will optimize the algorithm for these (> 100 pixels). The key is to use well-fitting data structure. Throughout the algorithm we perform two operations most often. The first one is .Contains(), which means 'does the specific pixel have a nonzero energy ?' and the second one is .Delete() with is setting the energy of a specific pixel to 0. An ideal option for these operations seems to be an array of 256x256 pixels which can effectively do both these operations in constant time. The problem is that this approach would lead to huge performance issues as most of the clusters are smaller than 100 pixels and the overhead of the array with 65 536 items would take much time. Using the list collection List<T> from the standard library, we get rid of this problem. On the other hand .Contains() and .Delete() take linear time to execute. That is why we chose to use HashSet<T> which has similar memory usage as List<T> but both .Contains() and .Delete() are done in a constant time. In case we would need another performance boost, the whole algorithm can be almost trivially parallelized.

## Filter and Description Generator

Both ClusterFilter and DescriptionGenerator calculate the features for many clusters, so we decided to analyze them together. The applications run on a specific collection for a potentially long time, so performace seems to be a reasonable factor we should try to focus on and optimize.

*Complexity*

The iteration process reuses ClusterInfoCollection and as we need to process every item in the collection, there is not much to be optimised. Let  denote the size of the px file and the size of the cl file. The iteration process has a linear time complexity with respect to . The calculation of an attribute value depends on the particular attribute. Asymptotic time complexities with respect to the number of pixels of a cluster is shown in the Table 4.1.

|  |  |
| --- | --- |
| ATTRIBUTE | ASYMPTOTIC TIME COMPLEXITY |
| PixelCount, ClIndex, PxFile, ClFile, Class | : All of these attributes are present when loading the cluster – no computational overhead |
| TotalEnergy, MaxEnergy, AverageEnergy, RelLowEnergyPixels, StdOfEnergy, StdOfArrival | : Calculation of these properties only requires an iteration over each pixel in the cluster, therefore we obtain the linear complexity. Because this is obviously also the lower bound, we can state that the complexity |
| Width, RelativeHaloSize, Convexity, VertexCount, CrossPointCount | : Because all of these attributes require skeletonization of the cluster, we need to analyze the Algorithm 1.1. Each iteration consists of pixels and there can be at most iterations, where is the thickness of the cluster. By analyzing the worst case scenario (cluster has a circular shape) we can notice that . When we combine these observations we obtain the resulting upper bound. (Note: Convexity and Width attribute require also convex hull calculation, which is done in , which doesn’t affect the asymptotic complexity) |
| BranchCount, Branches | originally, after update : When we look at the Algorithm 1.2, we can notice the following:   * The time clomplexity of the breadth first search[] is linear * The branch count could be at most linear with respect to the number of pixels.   Thus, we can estimate the worst case complexity by . In contrast, we usually do not need to analyze cluster much further if we already have hundreds of its longest branches. Because of that, we set the upper bound for branch count to be 40. We also set the depth of the calculation, so the algorithm ignores the branches that are nested more that four times. Even though this restriction doesn’t provide us a complete branch analysis, in most cases it is sufficient a provides significant performance boost to. (Note: From the real (non-asymptotic) observed calculation time it is still the most expensive calculation.) |

Table 4.1 Time complexity of the feature calculation

To sum up, the total complexity of the filtering process is , when taking the updated branch analysis into account.

*Adding new features*

To add a new feature to DescriptionGenerator, user needs to follow these steps:

1. Add the name of the attribute to the enum ClusterAttribute to the ClusterCalculator project.
2. Add a case to the switch section of the CalcAttributes method of the DefaultAttributeCalculator with your attribute and its calculation and store the value to the dictionary attributePairs to an index attribute. (attributePairs[attribute] = calculated\_value)
3. In the DescriptionGenerator project update the UI – add a checkbox to the other attributes with the same name as the name of the enum you added in the step 1 (because the string-enum conversions are done automatically).

## Classifier aplications

In this chapter we discuss the proces of cluster classifiacation from a developer point of view. We introduce some fundamental objects used in the classification proces, then we also mention a simple guild how to build your own classifier.

*Classifier objects*

**Interface IClassifier** –an interface which provides required methods for a classifier model (.Classify())

**Interface ILearnableClassifier : IClassifier –** an interface which extends the IClassifier by adding support for training (.Learn() method)

**Class NNClassifier : ILearnableClassifier** – a basic classifier based on a multilayered perceptron NN

**Class MultiLevelClassifier : IClassifier –** a classifier created by merging more NNClassifiers

**Class ClassPrediction –** an object that represents the prediction calculated by the classifier, apart from the name of the predicted class contains also the probabilities of how confident the classifier is about each class (implemented via the softmax function)

*Building your own tree classifier*

When you want to build a MultiLevelClassifier you first need to create a NNClassifier, which can be done two ways:

1. From the ClassifierUI
2. Using a console application ClassifierTrainer

After we have all of the NNClassifiers prepared, we can start with merging. There is a merging option in the ClassifierUI which only allows a single classifier on each level. In case you want to build any classifier tree, it can be done by following these steps (an example of how we merged our classifier can be seen in the .FromDefault() in the class MultiLevelClassifier):

1. Create new instances of NNClassifier and call .LoadFromFile() and create a new instance of MultiLevelClassifier
2. Wrap the simple classifiers into the class ClassifierNode and the root classifier into the ClassifierRoot
3. Connect the nodes starting from the bottom of the tree by calling parentNode.Descendants.Add(splitClass, sonNode)
4. After all of the previous steps are done, set the root by calling the method of the MultiLevelClassifier - SetRoot(classifierRoot)

*Serialization*

Each classifier that is created can be also stored in a file for the future use. This proces is called serialization and is done via the Newtonsoft library[]. When we were implementing the serialization of the both NNClassifier and MultiLevelClassifier, we needed to set all of the property modifiers to public so they can be visible for the serializer. Another problem is that the network itself (from the Accord.Net[] library), cannot be serialized using Newtonsoft[] library because of compatilibily issues. That is the main reason why as a result, each classifier is stored in two files (.csf and .csf\_support). The .csf file contains a serialized Network by the serialization tools of the Accord.Net[] library. In constrast the .csf\_support file contains the whole NNClassifier object except for the network itself (serialized by the Newtonsoft library[]).

*Selecting uncommon clusters*

One of the ultimate goals of the classification could be finding the uncommon clusters*.*Implementation of the selection of such clusters is implemented directly in the classification. ClassPrediction contains a method CalcConfidence(), which calculates the certainity of the prediction based on the output neuron values from the network. This method serves for detecting unclassified clusters. During the classification there is a method CheckSpecialClusters() is called which takes the unclassified cluster and decides if it can be considered an extraordinary cluster. Currently the implementation of this method only selects the clusters with nontrivial branch count and pixel count. Both CalcConfidence() and CheckSpecialClusters() are marked as virtual so they could be potentially reimplemented simply by inheritance. This is also where I see the biggest chance for improvement and extesion of the program.

# Experiment

During the work on the thesis, we created a few classifier models which need to be tested on the real datasets. For that we designed a few scenarios where we compare our approach with the alternatives and analyze the results.

## Even data distribution

In this section we decided to compare classificators trained on the datasets with evenly and also unevenly distributed dataset.

## Classifier Parametrization

## K-Fold cross validation of single-layered models

Because the training of the classifier is in general a non-deterministic procedure, we should also test the training method and how often is the classification training successful. Another property we might be interested in is variance of these results, which is precisely what we test in the experiment.

One of the most commonly used method for training evaluation is the k-fold cross validation[].

## Multi-layered classifier

A concept of multi-layered classifier is something we use in this thesis frequently. But how does it fare in comparison with a single layered classifier?

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**Epilogue / Conclusion**

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