

An Application of Visual Analytics Methods to Cluster and Categorize Data Processing Jobs in High Energy and Nuclear Physics Experiments

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Abstract

Hundreds of petabytes of experimental data in high energy and nuclear physics (HENP) have been collected by unique scientific facilities, such as LHC, RHIC and KEK. As the accelerators are being upgraded with increased energy and luminosity, data volumes are rapidly growing and have reached the exabyte scale. This leads to an increase in the number of data processing and analysis tasks, continuously competing for computational resources. The growing number of processing tasks requires an increase in the capacity of the computing infrastructure that can only be achieved through the use of high-performance computing resources. Along with the grid, these resources form a heterogeneous distributed computing environment (hundreds of distributed computing centers). Given a distributed model of data processing and analysis, the optimization of data and distributed data processing systems becomes a critical task, and the absence of an adequate solution for this task leads to economic, functional and time losses. This paper describes the first stage of a study which aims to solve the task of increasing the stability and efficiency of workflow management systems for mega-science experiments by applying visual analytics methods - data analysis leveraging an interactive GUI. That would allow to create specialized guidelines for pre-processing and brokering of computing jobs. Currently visual analytics methods are widely used in various domains of data analysis, including scientific research, engineering, management, financial monitoring and information security. Using data analysis tools that support data visualization, the information can be analyzed by an individual who is well-informed about the object of investigation, but who is not necessary aware of the internal structure of the data models. Furthermore, visual analytics simplify the navigation through



data analysis results: the data is represented by graphical objects, which can be manipulated either by mouse or using touch-sensitive screens. In this case human spatial thinking is actively used to identify new tendencies and patterns in the collected data, without having the users to struggle with underlying software.

In this paper we demonstrate visual methods of clustering computing tasks of the distributed data processing system using the ATLAS experiment at the LHC as an example. The interdependencies and correlations between various tasks or job parameters are investigated and graphically interpreted in an n -dimensional space using 3D projections. The visual analysis allows us to group together similar jobs, identify anomalous jobs, and determine the cause of such anomalies.

Keywords: visual analytics, high energy physics, nuclear physics, ATLAS experiment, cluster analysis

1. Introduction

HENP experiments generate vast volumes of data. As a result, HENP became one of the first scientific domains that faced the need for the processing and analyzing of exascale data and associated metadata.

The rapid growth and complexity of the distributed computing infrastructure of modern scientific HENP experiments as well as the exponential growth of the processed data volumes led to the emergence of new issues, whose solution can be significantly simplified with the use of visual analytics. Historically, the scientific experiments in the HENP domain used various visualization tools for data representation and for the different classes of tasks: detector functional simulation, the analysis of physics events, representing the results of research for information exchange within the scientific community. Such applications as HBOOK[1], PAW[2], ROOT[3], Ganglia[4], Geant4[5] have visualization tools which can be used for the purposes of visual data analysis.

In this paper we present the results of our studies of the metadata of the ATLAS experiment [6]. Information accumulated during many years of operation of the ATLAS data processing and analysis system (ProdSys2/PanDA [7,8]) contains data about the execution of more than 10 million tasks and 3 billion jobs (for more details about production system tasks and jobs see sections 2 and 3). The existing tools provide real-time control, monitoring and estimates of many parameters and metrics of the system. However, the current monitoring infrastructure does not have instruments for measuring the correlations among many different properties of the objects, as well as to analyze the time delays and its possible reasons during the execution of the computational tasks or jobs in the distributed computing environment.

In order to address these issues, visual analytics methods can be applied to derive new (implicit) knowledge about investigated data objects and to provide efficient interaction with data, relevant to the human cognitive system used for complex information processing.

In this paper we describe the cluster analysis of the computational jobs with the use of visual analytics methods. This is the first stage of the project of leveraging visual analytics for studying ATLAS distributed data processing system operations. This analysis will allow users to visually interpret the jobs with similar parameters by using 3-dimensional

projections and, at the same time, to monitor the correlations among different combinations of parameters.

2. The Distributed Data Processing System at the ATLAS experiment

The LHC experiments use computing Grid infrastructure that is provided by the Worldwide LHC Computing grid project (WLCG) [9], supercomputers and cloud computing facilities to process large amounts of data.

The second-generation ATLAS Production System ProdSys2 is designed to run complex computing applications, described by the concepts of computing tasks and jobs.

- A *task* contains the description of data processing applied to one dataset (a group of files with statistically equivalent events) in the ATLAS experiment, with processing parameters specified by the user/coordinator and the parameters describing the processing conditions. It also contains a “transformation” script to derive the output data files from the input files, and the version of the compiled software. Tasks are split into jobs that are then executed in the distributed computing environment. The results of task execution, i.e. the files, constitute the output datasets.
- ProdSys2 orchestrates the workflows of tasks, including the chaining of tasks that act in sequence on the same datasets. It manages tasks related to event simulation (event generation from physics models, detector simulation etc.) and to event reconstruction and analysis. Tasks are split into jobs that are then executed in the distributed computing environment. The results of task execution, i.e. the files, constitute the output datasets.
- The processes of creating chains of tasks, their fragmentation into jobs, scheduling jobs execution, and their launching on computing resources, are performed by ProdSys2/PanDA and are fully automated.
- A *job* is the unit of processing (i.e., “payload” for a computing node). The job record contains information on the input and output files, the code to be run and, after execution, the parameters of the computing node on which it ran and some performance metrics.

Currently (2018), the computational workload of the distributed data processing and analysis system ProdSys2/PanDA manages on an average 350K tasks per day in over 200 computer centers (totalling more than 300K computing nodes) by thousands of users [7]. Figure 1 shows that the system processes on an average 129 PB of data per month, while figure 2 shows the number of completed jobs, which is about 23.8 million per month. It is important to note that during the periods preceding important events (such as international conferences in HENP) the number of completed jobs reaches up to 2 million per day.

The scale of the system described above, its internal complexity, heterogeneity and distribution, as well as the volume of data processed requires non-trivial analytical tools to analyze and forecast the state of system functioning. The first step that needs to be done in this direction is the development of a toolkit that provides a convenient and understandable way of identifying correlations through data clustering; it will allow not just the use of various clustering algorithms, which are often represented as “black boxes”, but also provide the researcher with the opportunity to interact with clustering parameters and have a visual

presentation of their results. This will strengthen the human control over the analysis process of complex multidimensional data and make this analysis more meaningful.

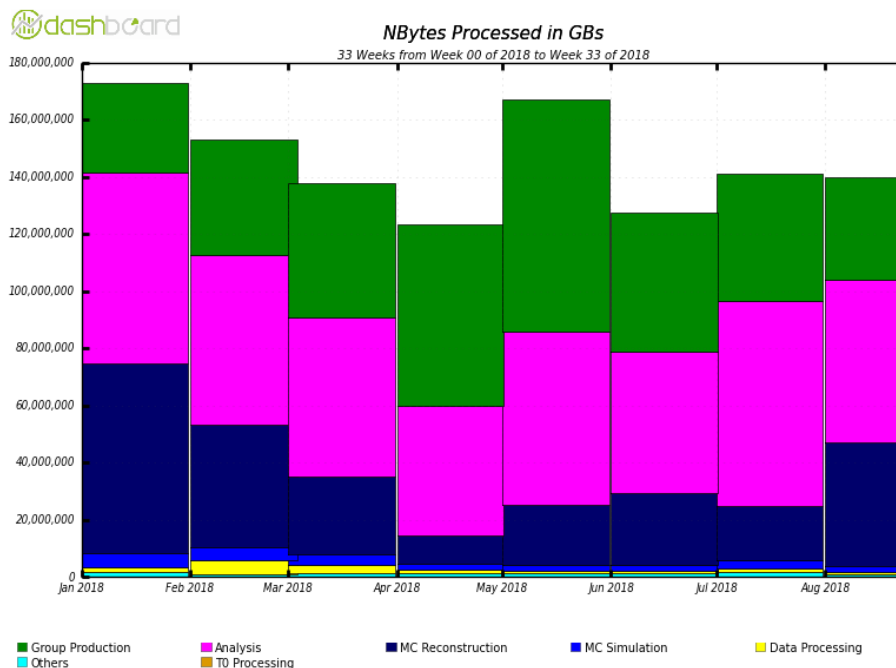


Figure 1. The volume of data processed by ProdSys2/PanDA in the ATLAS experiment from January to August 2018 as function of the job type

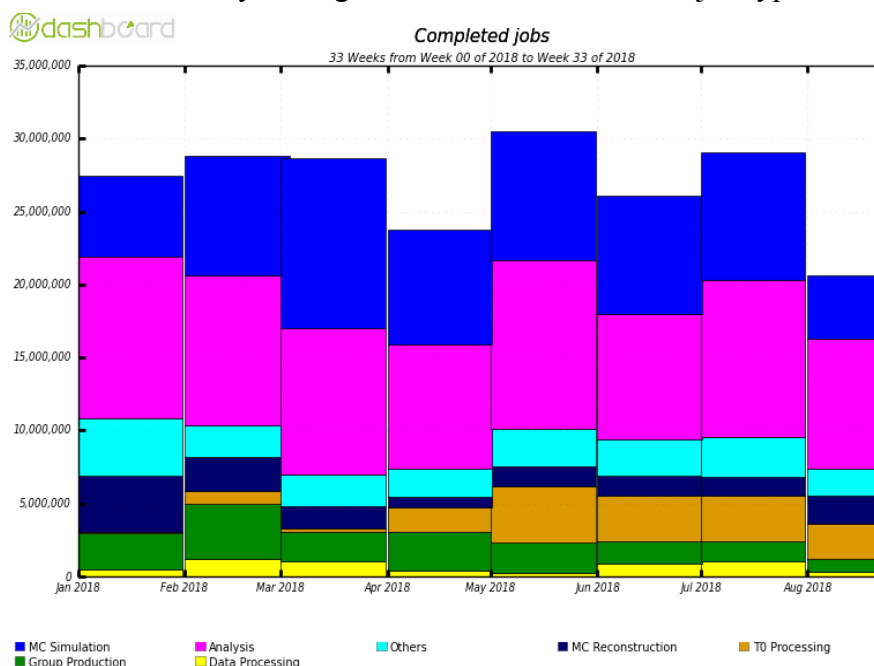


Figure 2. The number of completed jobs in the ATLAS experiment from January to August 2018 as function of the job type

3. Investigated Metrics of ATLAS Distributed Data Processing System Computing Jobs

The first stage of the research is searching for the relevant input data and its preprocessing for the further analysis. In our case we have chosen the performance metrics of

ProdSys2/PanDA jobs belonging to particular tasks. ProdSys2/PanDA keeps the state and all the running parameters of jobs in an Oracle database. Jobs themselves send monitoring information back to Oracle, from where it can be collected and preprocessed for subsequent analysis.

Following this we can generate the visual 3-dimensional projections of the values of the jobs parameters and analyze them. This allows exploring and understanding the progress of data processing for tasks as their jobs have the same executable code and the same size of the input data. The following test parameters that characterize the resource consumption were chosen to describe computing jobs:

- Task ID in ProdSys2/PanDA: **ID** (integer)
- Duration of the computing job execution: **duration** (integer)
- Volume of input data for the job: **inputFileBytes** (integer)
- Volume of output data of the job: **outputFileBytes** (integer)
- Processor efficiency (the ratio of total processor power times duration by the product of the job execution time by the number of cores): **CPU eff per core** (integer)
 - $cpu_eff = cpu_time / (wall_time * num_of_CPU)$
- Consumption of the processor time: **CPU consumption** (integer)
- Average size of memory pages allocated to the process by the operating system and currently located in RAM: **avgRSS** (integer)
 - Average portion of memory occupied by a process, composed by the private memory of that process plus the fraction of shared memory with one or more other processes: **avgPSS** (integer)
- Average size of the allocated virtual memory: **avgVMEM** (integer)

4. Visual Analytics Method for Cluster Analysis

In order to perform a cluster analysis using visual analytics methods, the sequential projections method was used [10]. This method was developed by the research group of MEPhI (“Scientific Visualization” laboratory) and its main idea is to transform the multidimensional data objects and the distance between them into geometrical objects. It allows the analysis of the data directly within the initial multidimensional space, without the need to use the dimensionality reduction techniques. This method was described in the “Scientific Visualization” journal [11]. The report was presented at the GraphiCon’2014 conference, and the article was published based on the conference materials [12]. The proposed method was tested on credit organizations’ data to distinguish those with anomalous characteristics [13].

The ProdSys2/PanDA computing job parameters were given as multidimensional tabular data. Then every row of this table was mapped to a point in multidimensional space E_n with the coordinates of points expressed as normalized parameters values: $p_i = (p_i^1, p_i^2, \dots, p_i^n) \in E_n$. In this work, the Euclidean distance between points $p(p_1, \dots, p_n)$ and $q(q_1, \dots, q_n)$ was chosen as the measure of differences between computing jobs p and q : $d(p, q) = \sqrt{\sum_{i=1}^n (p_i - q_i)^2}$. To evaluate the distance between n -dimensional points, the visual interpretation of those points is used.

The initial set of points is projected into a 3-dimensional spaces. Each multidimensional point p_i is projected to a 3-dimensional point, which then is represented as a sphere S_i (using the central perspective, that is, all the other coordinates, besides those three in use, are equated with zero). A graphical projection of the obtained spatial scene is presented to the user (Figure 3). Thus, the user has tools to control the image and the spatial scene (affine transformations, gathering the information about the points corresponding to spheres).

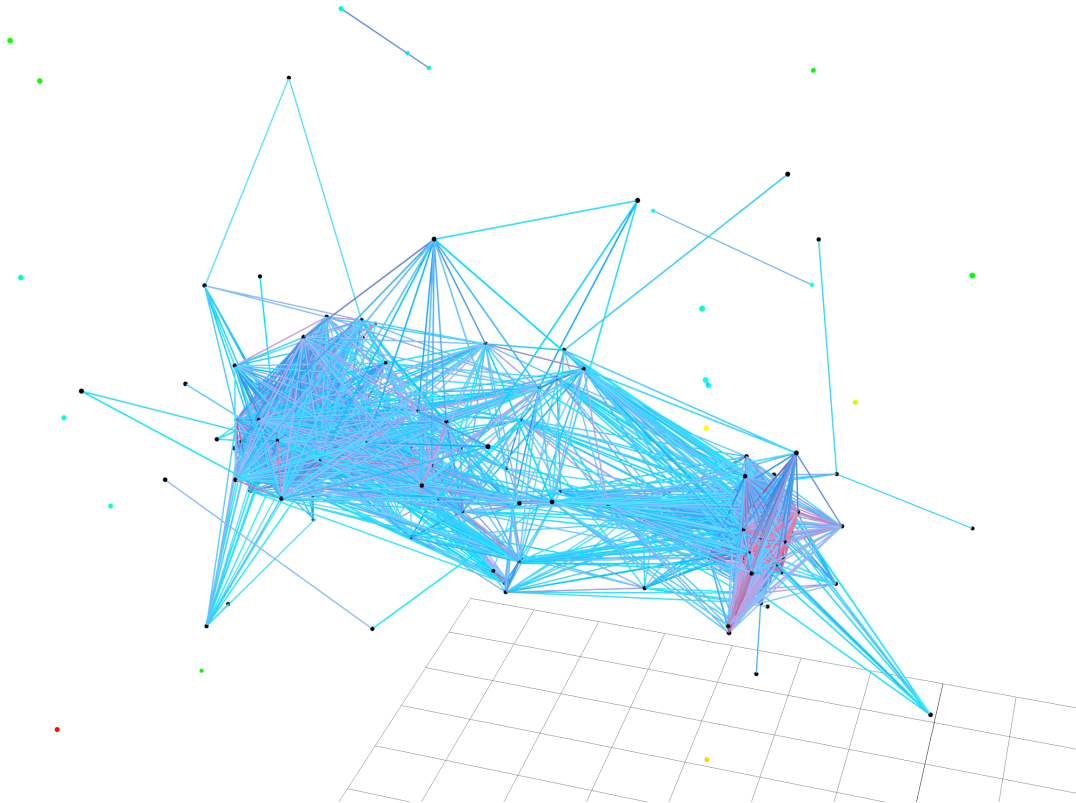


Figure 3. Spatial scene projection

For visual representation of objects connectivity the threshold distance d (*the maximum distance inside the cluster*), given by the analyst in an interactive mode, is used as shown in Figure 4. If the distance between n -dimensional points is less than d , points are connected with a segment, visualized as a cylinder, the color of which changes from red (the distance is small) to blue (the distance is close to d). The groups of connected points form clusters. Separate points, located far from all other points in the multidimensional space, represent the anomalous data points that will be the object of more detailed investigations.

Thus the visually observable presence of cylinders between spheres allows the analyst to visually capture the closest points in space, forming a cluster, and corresponding to them closest source objects, also forming their own clusters. Assigning different colors to cylinders allows to make judgements about the distance in the multidimensional space by only observing a 3-dimensional spatial scene.

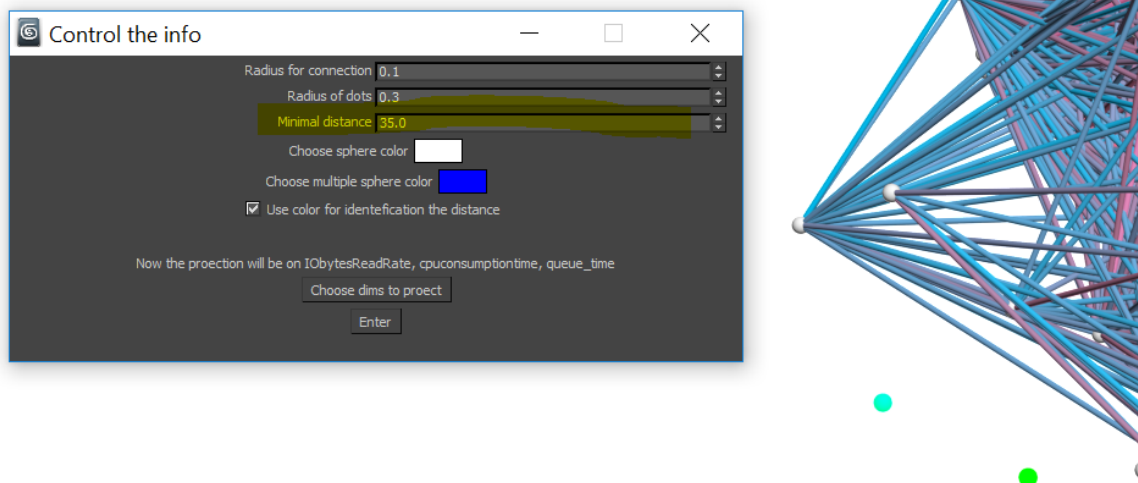


Figure 4. Control window of geometrical and optical parameters.
The threshold value d is marked in yellow.

5. Software Implementation of the Visual Analytics for Cluster Analysis

Scientific papers analysing the description of specific applications using visual methods suggest that interactive systems working with multidimensional data are often given less importance than the results representation systems which use Data Analysis methods. For example, there are systems such as the AdAware situational alert system [14], the visual analysis system in aircraft tasks [15] and the SAS Visual Analytics software package [16], designed to handle and analyze large volumes of financial and economic information. All these systems are industrial and commercial. They provide to the users a huge number of interfaces and possibilities of visual representation of the data. At the same time, there are no publications on the use of such systems in the field of particle physics. As practice shows [17, 18], the classical methods of parallel coordinates, Andrews curves, faces of Chernov [19] and other similar mnemonic graphic representations are widely used for such visual representation of multidimensional data. All these visual methods are based on the fact that the analyzed tuples of numerical data are interpreted as values of parameters of such mnemonic graphical representations.

However, the majority of the visual analytics systems are tuned to the internal processing of data and its representation in a form suitable for the user. These systems do not allow the user to interact directly with the visual representation of multidimensional data.

The above method of clustering analysis of multidimensional data was implemented in an application named IVAMD (Interactive Visual Analysis of Multidimensional Data) [20]. This application allows users to interact directly with the initial n -dimensional data. These data are not preprocessed. The analyst manipulates the initial data in a targeted way providing the visual analysis of the obtained results.

IVAMD was written in MAXScript¹ and a module written in C#. Its main functionality includes displaying a spatial scene using customizable visualization parameters (threshold distance d , radius of the spheres and cylinders, three-dimensional subspace for projection), performing affine transformations of the three-dimensional space, calculating the distance in the original n -dimensional space, splitting into clusters (clusters are denoted with colors), and conducting the microanalysis (2-dimensional scatter plots) of the spaces. In the microanalysis, that is the analysis of distant points, it is important which coordinates make a greater contribution to the distance - whether it is due to all the coordinates or due to the large difference of only few coordinates. To determine this, graphical projections of the original set on the plane (x_i, y_i) are built and then all these projections are viewed for different values of i . The results of clustering can be seen while using the program, and they can also be exported to an Excel spreadsheet marked with different colors, corresponding to the clusters and anomalous points. An example of such a table is shown in Figure 5.

ID	avgpss	avgrss	avgvmem	cpu_eff	cpuconsumptiontime
378	3,02155	0,540255	0,0968087	0,340742	5,01355
2219	0,710337	0,134811	0	0,370008	6,94845
2460	1,59649	0,263486	0,35708	0,129835	5,43723
2463	1,44083	0,17454	0,268137	0,391832	6,4773
2494	1,40164	0,146246	0,230384	0,25998	7,76454
2510	2,00695	0,575056	0,115821	0,286225	7,20546
7700	47,9374	45,687	49,1948	51,373	23,8059
9437	44,9547	45,6759	49,3565	51,3017	23,6733
9438	46,4195	45,9381	49,5506	51,662	26,3812
10219	47,1236	45,9035	49,7007	51,6055	26,4637
10220	45,6879	45,6556	49,1678	51,2164	26,7734
10371	49,3227	46,2934	49,647	51,2322	29,2729
10976	97,9758	99,5828	99,5562	80,0312	72,2983
11007	99,2486	99,502	99,3153	100	74,6276
11247	1,22865	0,305296	0,335525	0,438041	39,7412
11272	1,49591	0,337036	0,426979	0,116061	46,876

Figure 5. The resulting table with color highlighting of clusters and anomalous objects

Due to the peculiarity of the method, the necessary number of objects for visualization to solve the problem (m rows, n columns) is m spheres (equal to the number of rows) and the number of cylinders is equal to $m \times (m - 1) / 2$. Resulting in $m \times (m + 1) / 2$ objects to display; such that to display 100 lines, it is necessary to display about 5050 3DSMax primitives. The described software is a prototype of the implementation of the method and has a limit on the number of processed objects. Further development and improvement of the prototype, and optimization within the framework of high-performance hardware and software infrastructure will eliminate the current limitations.

The main advantage of this software prototype is the interaction between the user and both the data and the spatial scene. Changing the threshold distance iteratively, the researcher can visually investigate the changes in the cluster data structure, track the state of anomalous data objects like becoming abnormal at some threshold distance. In addition, all spheres of the spatial scene are clickable, allowing the user to see their multidimensional coordinates at any

¹ <https://marketplace.visualstudio.com/items?itemName=atelierbump.language-maxscript>

time. It allows the researcher to estimate which coordinates make the greatest contribution to the formation of clusters.

6. Applying the Visual Analytics Method

To test the method, a visual analysis of computational tasks consisting of dozens of jobs was performed. For example, task number 12196428 from the data collected on 02-10-2017 consists of 74 jobs. The first step was a macro analysis of the entire subspace, i.e. the original 7-dimensional space was clustered. The three-dimensional projection was made on the subspace: avgPSS, duration, outputFileBytes (presented in Figure 6). The results consist of 6 clusters (with a multiplicity of 31, 17, 8, 5, 3 and 2) as well as 2 disconnected points (clusters with a multiplicity of 1).

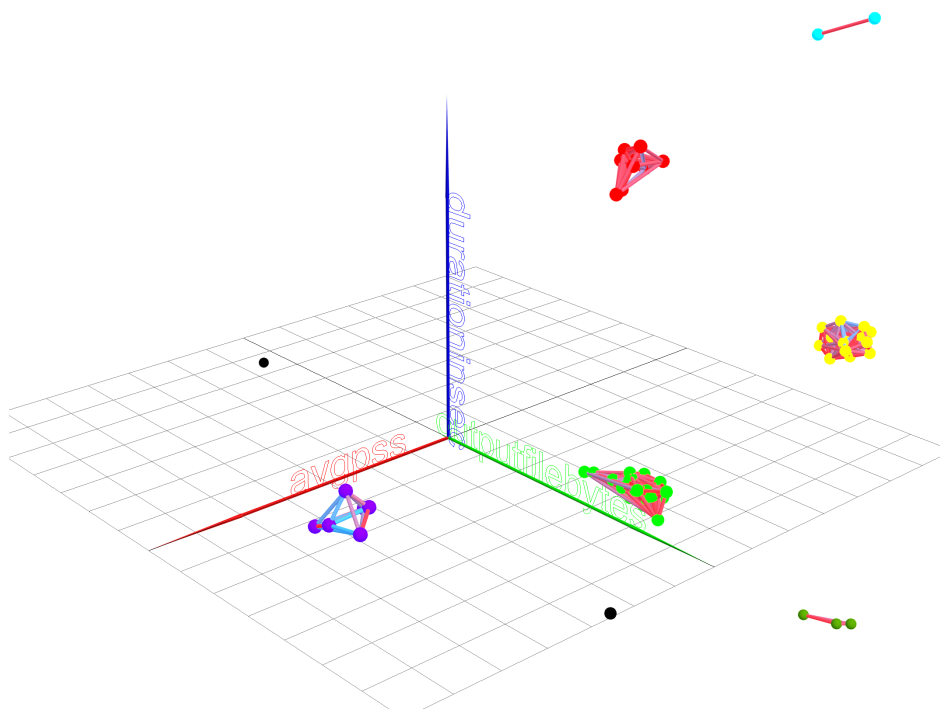


Figure 6. Partitioning into clusters in a three-dimensional projection (red axis - avgPSS, green axis - outputFileBytes, blue axis - duration in sec)

Next, a microanalysis was carried out to determine the contribution of various parameters to partitioning into clusters, as well as assessing the influence of various parameters of objects on the duration of the execution of computational tasks.

In Figure 7, one can see that with the same avgPSS, the difference in duration between the red and green clusters is significant. A similar pattern is observed for the avgRSS and avgVMEM parameters, which allows us to conclude that the listed parameters contribute to the duration of the tasks, but only at moderate values. This relationship requires additional research on more points.

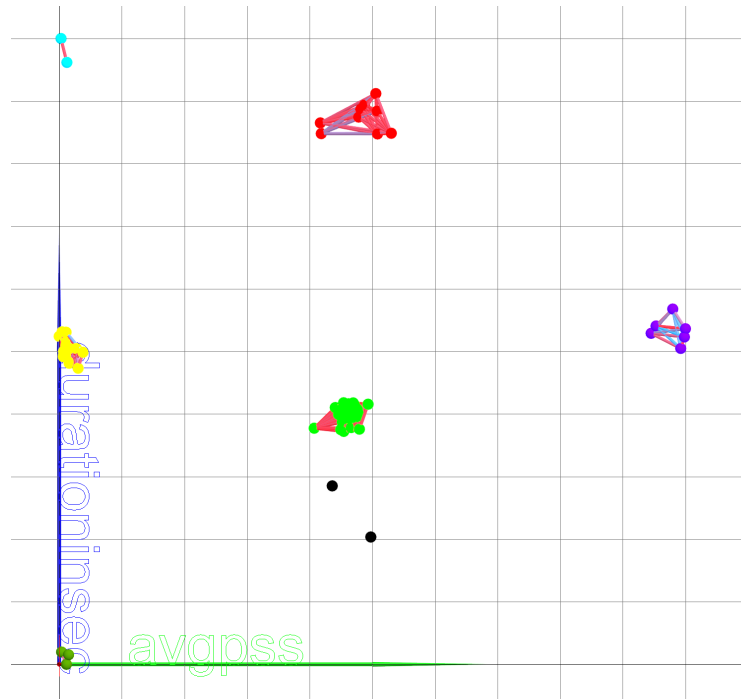


Figure 7. Graphic projection on the plane (avgPSS, duration)

In Figure 8 it can be seen that the difference in CPU consumption is directly proportional to the duration, as expected.

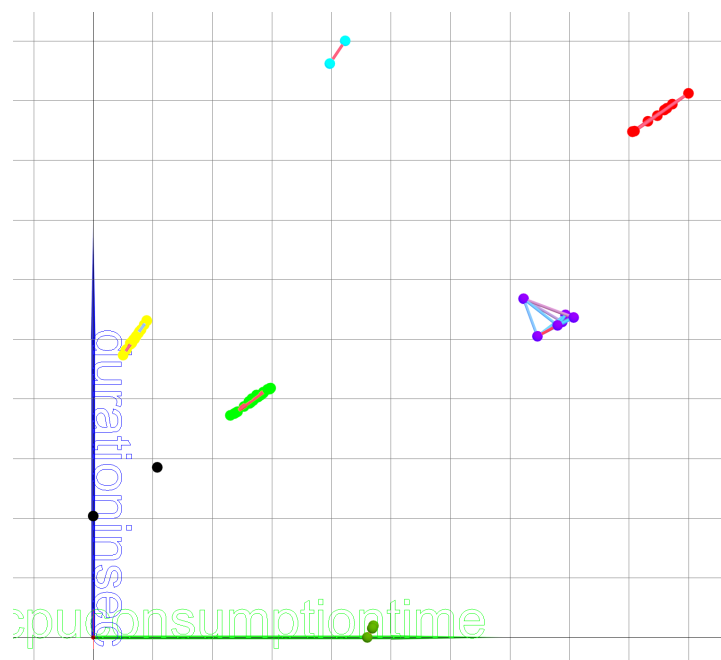


Figure 8. Graphic projection on the plane (cpuConsumptionTime, duration)

Figure 9 shows that the degree of influence of the input file size (inputFileBytes) on the duration of processing and analyzing data is not decisive for distributed processing. This also applies to the output data files (outputFileBytes) as it is shown on figure 10. To quantify the impact of data volume on the duration of the tasks, additional research is needed on more statistics, which will be carried out in the future.

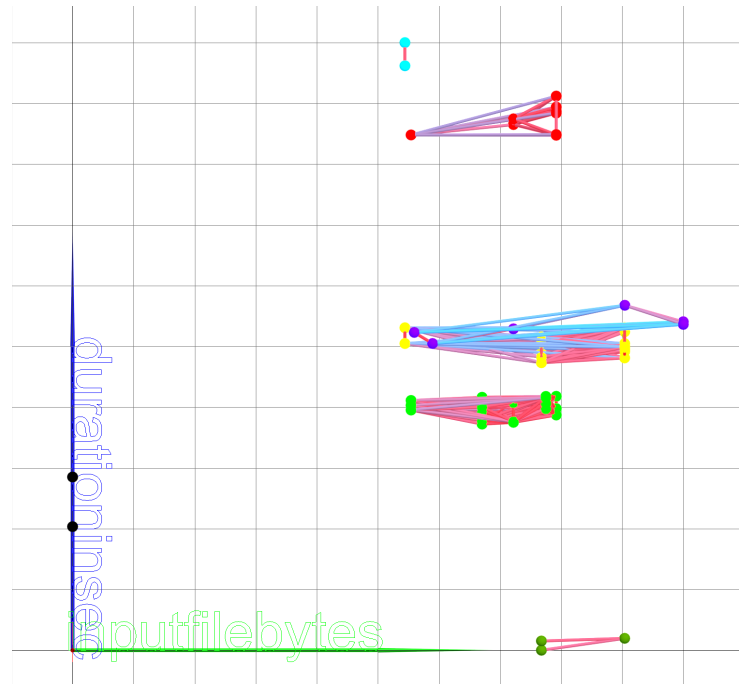


Figure 9. Graphic projection on the plane (inputFileBytes, duration)

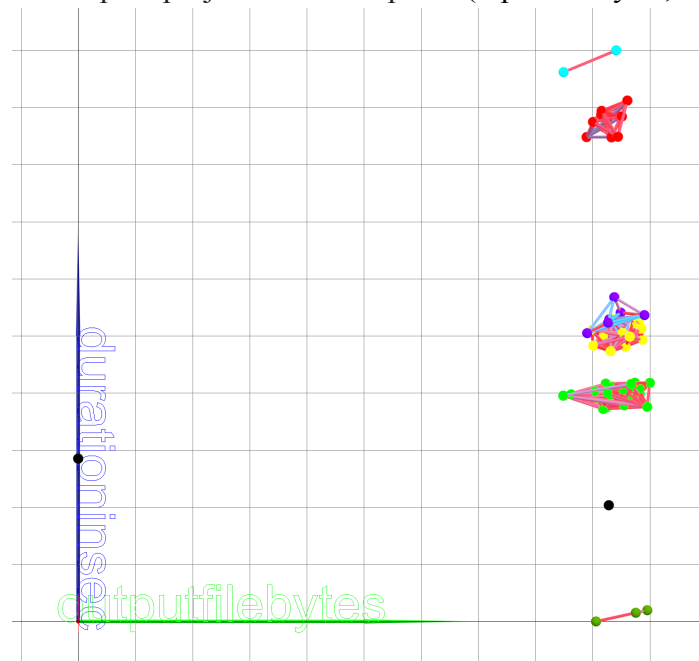


Figure 10. Graphic projection on the plane (outputFileBytes, duration)

7. Conclusions and outlook

This work is the first attempt to apply visual analytics methods to the analysis of ATLAS distributed computing metadata. Due to great amount of data and its complexity and multidimensionality, the existing Machine Learning and Statistical methods of data analysis need visualization tools, allowing to increase the human supervision of the analysis process. This paper demonstrates the method of visual analysis through clustering and categorization applied to jobs of the ATLAS distributed data processing system. This method is based on the

geometrical representation of multidimensional data in 3-dimensional space in form of spheres with precalculated n -dimensional distances between them. The closest spheres are connected with segments, forming clusters. The analyst interacts with the spatial scene, change the distance threshold and observe the changing structure of the clusters.

As further development it is planned to implement a multi-layered model of interactive visual clustering. This model implies the concept of Superpoints: as the initial data samples can be too large to have all data points visible, the visual representation can be reduced by using Superpoints, which are collections of similar points [21]. Superpoints are computed using clustering algorithms and constitute the first layer. Each Superpoint can then be analyzed separately as the collection of its data objects, leading to the next layer of clustering. Furthermore, it is planned to refine the visual analytics platform with the ability to interactively switch among different layers of clusters. In this way the researcher will be provided with a convenient method to interpret the results of clustering based on different levels of data granularity.

The results can be used for the visual monitoring of ATLAS distributed data processing system as well as for the implementation of optimisations of the jobs execution time.

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