

Optimizing Material Data Management and Analysis Using Engineering Web Applications

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Abstract – The development of technological devices has been accompanied by a significant increase in the generation of data, as well as the evolution of terminology and formats used to store it. In the past, data was typically stored in a variety of formats, such as relational databases, Excel, .hdf5, .xml, .csv, .docs, .rtf, .odf, and others, each offering distinct methods of data organization. Among the most complex types of data are material data, which are crucial for engineers when performing analyses and designing experiments. Engineers can leverage this data to manipulate it in ways that answer specific questions posed by a company or solve particular challenges, enabling them to recycle and reuse data efficiently. However, with the rapid advancement of technology, accessing older file formats has become more challenging. To address this, web applications have emerged to manage and store material data more effectively. These platforms allow engineers to perform statistical analyses while optimizing the storage, recycling, and management of material data.

The objective of this paper is to provide a comprehensive review of existing academic and scientific literature on material data. It will also include a survey targeting engineers to identify the best practices for storing material data, based on its type, physical properties, mechanical characteristics, and standard classifications. Furthermore, the paper will explore how material databases are structured and demonstrate the process of reading large hdf5 files using Django and Python, with a focus on achieving optimal performance.

Keywords – Material Data, Recycling, Unstructured Data, Hdf5, Engineering, Optimizing, Resources, Physical Characteristics, Mechanical Properties.

I. INTRODUCTION

Data plays a very important role, especially with the continuous growth of technology, and among these data, material data can be specifically mentioned. These data are usually more commonly used by engineers and various companies who focus on them for conducting analyses or scientific studies, as well as for deriving solutions to specific problems.

Material data refers to information about the materials used, which serve as sources for engineers or manufacturing companies to conduct various statistical or scientific analyses. These data describe the characteristics, physical properties, and mechanical properties of materials. Another definition of material

data according to Abaqus is that any material definition can contain a number of material behaviours, as required, to specify the full behaviour of the material [1]. Each material definition must be assigned a name. This name allows the material to be referenced by section definitions used to assign this material to the regions of the model.

Material data can be considered as one of the most complex types of data because they are used by engineers or companies for analysis and experimental design. This means that these existing data can be used to manipulate and derive important solutions depending on the problems or questions that may arise from manufacturing companies.

The reasons why digital access to material data are important:

1. **Automation of Product Design and Engineering** refers to the increasing use of computer-assisted engineering in all stages, from planning and design to manufacturing and distribution, utilizing advanced software and devices. Significant progress has been made in integrating individual tools into comprehensive systems, enabling seamless data transfer between activities with minimal loss of quality. Although the engineering integration process is not yet complete, manufacturing and production are moving toward becoming fully integrated and diverse in today's global environment.

2. **Ease in building Material Databases:** The advent of information technology has made managing material data easier, but challenges remain with fragmented databases, making it hard for users to access integrated data on materials like ceramics, metals, and plastics. As an example, a recent study of ceramic property data sources identified over 100 individual sources, none of which are integrated together [2], and there is no current directory that lists these databases.

3. **Maturity of Material Modelling:** Physics-based modelling requires data for validation, but progress is limited by the lack of comparison with experimental data and the poor integration of modelling tools and databases. While some fundamental data exist, essential modelling data are often unavailable or not shared. Full benefits of material modelling will only be realized when such data are more accessible.

4. **Use of Big Data and Information in Materials Science for the Development of New Knowledge:** Big Data is defined by volume, velocity, variety, and veracity, with variety and data quality being most important for material data. The rise of Big Data has increased the visibility of data activities, and advanced tools like machine learning and data-driven approaches are becoming more common. These methods are crucial for extracting meaningful insights in materials science, requiring complete and accurate datasets.

5. **Emergence of New Materials and the Need for Accelerating Their Adoption:** New materials are rapidly emerging, but a lack of accessible data hinders their adoption in products. Improved data availability is crucial to accelerate the adoption of these materials in manufacturing.

There are also five types of material data that have emerged as a result of a study of 50 common characterization techniques and modelling techniques. These are: scalar data, time-series data, spectral data, categorical data, and image data [3]. By categorizing these data, the goal is to identify distinguishing techniques that can be easily transferred to other measurement modules that produce similar material data classes. These categories help in understanding how different data types can be used effectively in materials science for modelling and characterization purposes.

II. MATERIAL DATABASE

A materials database is a database used to store experimental, computational, standards, or design data for materials in such a way that they can be retrieved efficiently by humans or computer programs [4]. Engineering materials databases are the basis of materials informatics, manufacturing industries and the related disciplines [5]. Design and development of materials databases is done to enrich the availability and accessibility of materials data to materials scientist, researcher and design engineers in manufacturing industries [6]. Many manufacturing industries have organized material data into databases, which are accessed to search for and verify materials that meet design requirements. The International Atomic Energy Agency (IAEA) has created a database of natural matrices that is internationally available as certified reference materials (CRM). This database is frequently accessed and periodically updated, but its access is limited to the developmental work of the IAEA [7].

Material databases store information measured by researchers or technicians concerning materials and their use avoid repeated experimental measurements. Material databases obtain information through their own experimental tests, like Granta (ANSYS) [8] and Altair material data center [9], or through scientific papers, which is done by MatWeb [10] and MatDat [11].

The final purpose of material properties databases is to provide trustful information on a material and avoid repeated measurements and their inherent costs. Considering that, nowadays, everything is designed using simulation tools that require material information for their constitutive models [12], the information provided by material databases becomes vital. Today, the majority of the solid mechanics simulation tools which consider the material macroscopic behaviour, perform a Finite Element Analysis (FEA), a method of simulating real material behaviour on computers that utilizes the Finite Element Method (FEM) [13].

Key features of a material database may include:

1. **Physical Properties:** Characteristics like density, thermal conductivity, electrical conductivity, and melting point.
2. **Mechanical Properties:** Information such as tensile strength, hardness, elasticity, and fatigue resistance.
3. **Chemical Composition:** The elemental makeup of materials, including purity and alloy composition.
4. **Performance Data:** Information on how materials behave under stress, temperature changes, and environmental exposure.
5. **Manufacturing and Processing Data:** Data on the material's processing methods, such as casting, extrusion, or additive manufacturing, and any limitations or benefits tied to those methods.
6. **Environmental Impact:** Sustainability aspects, such as recyclability, carbon footprint, or biodegradability.

Material data can be stored in various formats depending on the use and system requirements:

1. **Text-based formats (CSV, TSV):** Simple, tabular data storage, easily imported into analysis programs.
2. **XML and JSON:** Used for hierarchical and structured data, with JSON being more common for web applications.
3. **Database formats (SQL, NoSQL):** SQL for relational data and NoSQL for unstructured or semi-structured data, offering flexibility for large datasets.
4. **Modelling formats (STL, STEP, IGES):** Used for storing 3D models of materials and product parts.
5. **Performance data formats (CSV, HDF5):** Useful for storing experimental and performance data, with HDF5 handling large, structured datasets.

The choice of format depends on the specific application and how the data will be used.

III. RECYCLING MATERIAL DATA

A. Data recycling

Data recycling refers to the practice of taking old data that was originally collected to solve a specific problem and repurposing it to draw conclusions about newer issues, until companies gather direct data that either confirms or refutes the findings from the recycled data.

Often, data recycling is also referred to as data reuse, especially when different departments within a company use the same data to achieve different goals. This process can be a valuable opportunity for companies, as recycled data can serve various purposes, one of which is scientific research. A common argument for data sharing is to avoid duplication of research effort, thus accelerating the pace of science [14]. Reuse thus implies usage of a dataset by someone other than the originator [15].

The lack of access to data often creates difficulties for researchers in conducting comparative analyses, particularly when the data they have comes from only one specific region of the world or is not sufficient to make accurate comparisons.

Companies may choose to recycle their data when they are confident in its validity and accuracy and believe the information can help analysts draw multiple conclusions from the available data. When this happens, data analysts can shorten the time needed to solve a problem, as they can use the findings from

one dataset to help answer other questions, achieving more efficient and quicker results than would be possible without that information.

B. The Role of Data Recycling Applications in Business

Businesses are increasingly struggling with data accumulation. After years of viewing data as essential, many organizations, especially smaller ones, now face the problem of having more data than they know how to manage. Much of this data, though often considered “waste,” still holds value. Just as physical materials are recycled, the same approach should be applied to digital data. However, many companies have yet to adapt this mindset, leaving teams to sift through digital clutter, slowing down their work and making the search for useful information frustrating.

It’s time to adopt data recycling practices. By identifying and repurposing valuable information, companies can improve collaboration, knowledge sharing, and productivity. Digital data recycling helps overcome the challenges of information overload, ensuring that businesses don’t face macro threats to productivity.

Sorting and organizing data is the first step. Like separating recyclable materials, we need to distinguish useful data from irrelevant or outdated information. This is crucial since much data is created for specific tasks and doesn’t need to be kept forever. Retaining it only hinders the discovery of essential information.

Artificial Intelligence (AI) can assist by building knowledge networks that recycle raw data, adding context and transforming it into valuable resources. A self-learning knowledge network can combine information to make it more useful. AI helps by sorting out outdated data, analysing broader contexts, and identifying what’s needed, presenting it in an actionable way. When existing knowledge networks don’t provide answers, AI can help identify the best person to solve a problem by analysing all available data, since much knowledge remains undocumented and stored in people’s minds, AI can connect experts with individuals needing answers in real time. Once shared, the information is added to the centralized knowledge network for future use.

The transition to online material databases enhances global collaboration, reducing costs. By embracing the right technologies, businesses can maximize the value of their data, streamline operations, and focus on what truly matters, solving problems and sharing expertise across the organization.

C. Data Recycling Applications

Some applications that are used from company for data recycling:

1. EDA is a platform that integrates data management, modelling, and knowledge management to support materials engineering. It offers flexible data handling, processing, and visualization, enabling the entire material information lifecycle. EDA can interface with testing systems, CAE, CAD software, and other tools, covering workflows from data collection to parameterizing material models. These models can then be exported to CAE applications like Abaqus and LS-Dyna [16].

2. Matmatch provides a comprehensive database of metals, polymers, composites, and ceramics. It is free to use and offers a powerful search tool that allows users to find materials by name, type, or property. The database includes chemical, mechanical, thermal, electrical, and optical properties for thousands of materials, including commercially available materials from suppliers, and is regularly updated with new data., Users can contact with suppliers directly through the platform to inquire about materials [17].

3. Material Connexion offers a rich database of polymers, glass, ceramics, cement-based materials, carbon, and metals, complete with detailed physical or mechanical performance data and availability. The only requirement is that you must apply for membership before accessing the database [18].

4. Material Web is a large database of structural, electronic, and thermodynamic data for materials in 2D or 3D formats. It includes a powerful API that allows you to write Python code to help characterize any material. While aimed primarily at researchers and developers, it remains an excellent tool for material exploration once you’ve registered on the platform [10].

5. Materials Project is an interactive exploration platform suitable for both casual browsing and educational purposes. The database includes individual categories for batteries, crystals, and molecules. Primarily focused on exploring and evaluating the physical properties of various materials, this platform holds particular practical value for specific engineering fields. Materials Project offers the ability to search

for material information based on chemistry, composition, or properties of metals. The platform also enables the generation of phase diagrams and Pourbaix diagrams to identify stable phases and study reaction pathways. You can design new compounds using their structure editor and substitution algorithms. Additionally, it allows you to calculate the entropy of over 10,000 reactions and compare them with experimental values [19].

6. MatWeb is a large material database categorized by physical properties, alloy composition, material type, manufacturer, name, or UNS number. It is especially useful for those looking for materials that are released and actually used in the market, containing over 120,000 entries. It offers: quantitative searches, categorized searches and text search based on your interest.

7. MatDat is another material database focused on engineering, containing over a thousand data sheets for steel, aluminium, cast iron, and titanium alloys. The results focus on practical engineering, offering mechanical properties in beautifully formatted and downloadable PDFs. Notably, MatDat's search features allow visitors to filter by standards such as ISO, SAE, and ASTM for precise material identification.

D. Use of Material Data Recycling Techniques in Albania

"Material data recycling" is a technique widely used and well-known in developed countries, but in Albania, this concept is relatively unknown. To assess the awareness of this technique, we conducted a simple survey with technology experts, including individuals in these positions: Software Developer, Software Engineer, Team Leader Software Engineer, Quality Assurance Tester, Python Developer, etc.

If the survey had included individuals from other fields, particularly engineering, the data could have been more accurate. However, due to challenges in finding people from these fields, we decided to conduct the survey only with technology experts. The goal was to understand the awareness of the "material data recycling" concept. Based on the survey results, it can be concluded that employees in technology companies are not very familiar with this concept.

One of the questions in the survey was: "Have you heard of material data recycling before?", figure 1.

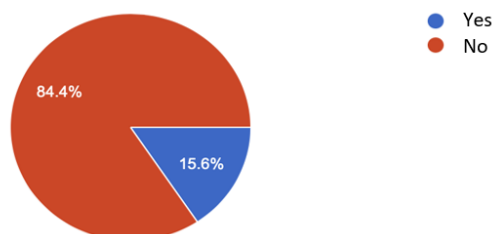


Fig 1: The result of on question in the survey in Albania

Those who had previously heard of the concept were fewer, and as shown in the graph above, only 15.6% of the interviewees have heard of it. They have not used any application for data recycling before; they are simply familiar with the concept.

The interviewees were also asked if they knew of any companies in Albania that use such an application or have developed one for material data recycling. The responses were negative, meaning they were not aware of any such companies in Albania.

IV. THE TOOLS AND TECHNOLOGIES USED FOR A DATA RECYCLING APPLICATION

To develop an application for data recycling there are several tools:

1. Python is a versatile, high-level programming language known for its readability and simplicity. It supports multiple programming paradigms, such as procedural, object-oriented, and functional programming. With a vast standard library, Python is one of the most popular languages used for various applications, including data processing and machine learning [20].

2. Django is a high-level Python web framework that promotes rapid development and clean design. It simplifies web development by handling many common tasks, allowing developers to focus on creating the application rather than dealing with repetitive work. Django is free and open-source [21].

3. SQL (Structured Query Language) is the standard language for managing data in relational databases. It is essential for organizing and querying large datasets efficiently in data-intensive applications.

4. Machine Learning (ML) is a field of artificial intelligence that focuses on algorithms that use data to improve performance without being explicitly programmed. ML is widely used in applications like predictive analytics, email filtering, speech recognition, and computer vision. It builds models based on training data and is particularly useful for tasks where traditional programming approaches are insufficient [22].

5. Excel is a widely used tool for data manipulation and analysis, but it is suitable for simple tasks.

6. HDF5 is ideal for storing large sets of homogeneous numerical data, organized hierarchically with metadata. It doesn't support complex relationships like JOINS. It's excellent for high-performance, partial input/output tasks but less suitable for small data sets or relational features [23].

7. JSON is a lightweight data exchange format, easy for humans to read and write, and for machines to process. It is independent of programming languages and is perfect for data exchange [24].

A. Advantages and Disadvantages of material database

In this section, we discuss some of the advantages and disadvantages of applications using material databases, commonly employed by engineers and analysts for research and analysis. Some of the key advantages are:

1. Improved Data Sharing - These applications facilitate better access to well-managed data, enabling end-users to respond quickly to changes in their environment.

2. Enhanced Data Security - With increased access to data, the risk of data breaches grows. These applications provide frameworks to enforce better privacy and data security policies.

3. Better Data Integration - Wider access to well-managed data promotes an integrated view of organizational operations, making it easier to see how actions in one segment affect others.

4. Minimized Data Inconsistency - Data inconsistency occurs when different versions of the same data appear in multiple places. Properly designed databases significantly reduce the probability of data inconsistency.

5. Improved Decision-Making – Better managed data and enhanced access allow for the generation of high-quality information, which leads to better decision-making. The quality of decisions depends on the accuracy, relevance, and timeliness of the underlying data.

6. Increased User Productivity - The availability of data, combined with tools that transform it into actionable insights, empowers end-users to make faster and more informed decisions, which can distinguish success from failure in the global economy.

Disadvantages:

1. Increased Costs - Material database systems require sophisticated hardware, software, and skilled personnel, leading to high maintenance, training, licensing, and compliance costs.

2. Management Complexity - Implementing a database system impacts company resources and culture. Changes must be carefully managed, and ongoing security assessments are needed due to the critical nature of the stored data.

3. Frequent Updates/Upgrades - Database providers frequently release updates with new features, often requiring hardware upgrades. These updates incur costs and require additional training for users and administrators.

B. The Future of Material Data Recycling Techniques

Artificial Intelligence (AI), especially robotic classification, is transforming material data recycling and material discovery. AI enhances automation and accelerates productivity by learning from large data sets and building predictive models, offering a faster alternative to traditional trial-and-error methods. Unlike computational chemistry, where computers simply follow expert-coded formulas, AI autonomously identifies patterns and predicts material behaviour.

AI is revolutionizing material science by improving material design, performance prediction, and synthesis. With the vast amount of material data being underutilized, AI helps extract valuable insights and accelerates innovation. Machine Learning (ML) is rapidly advancing in material science research, enabling better prediction of properties, process optimization, and material characterization.

C. The Role of AI in the Discovery of New Materials

In recent years, Artificial Intelligence (AI), especially Machine Learning (ML), has significantly advanced material research, particularly in the synthesis of new materials and predicting chemical processes. ML models help bridge the gap between material design, synthesis, and processing by accurately predicting material properties and structures before actual synthesis.

For example, a study used an ML model in MATLAB to predict solid electrolyte materials from over 12,000 materials. By utilizing atomic structure data and applying "intelligent" features based on existing physical knowledge, the model predicted 317 potential materials. The results showed that ML's efficiency in identifying new materials was three times higher than random guessing and twice as efficient as human researchers in similar fields [25]. This approach reduces the need for numerous experiments, selecting the best-performing materials from a wide range of options and accelerating the process of material discovery and innovation.

V. DATA RECYCLING IN BUSINESS, VISUALIZATION OF THE HDF5 FILE

Data recycling is one of the most crucial and effective processes for businesses. It establishes a network of knowledge and ensures the uniform distribution of information among employees within a company. Storing all this information in a shared database used by various applications enables employees across the organization to share a common perspective, ensuring consistency of standards throughout the company.

A. Functional requirements

The functional requirements of the systems will be: The users will upload the hdf5 file and the application is designed to read an HDF5 file containing thousands of records related to material data, making the process of analyzing this data easier for engineers and analysts. Furthermore, the application allows the processing of these data for different datasets and presents the data in 2D graphical formats. Additionally, it offers the option to download the graphical representation for further analysis or reporting purposes.

B. Tools and Technologies used

The main technology used for development is the Python programming language. This technology was chosen for several reasons, with one of the key features being Python's extensive collection of libraries and modules. Python is also known for its simple syntax and fully supports object-oriented programming, structured programming, and many of its features support functional programming and aspect-oriented programming.

One of the packages Python offers, which was used for reading HDF5 files, is h5py. This package allows for efficient reading, writing, and manipulation of HDF5 files, making it ideal for handling large datasets typical in material data applications.

The h5py package is a Pythonic interface to the HDF5 binary data format. It allows for efficient storage of large amounts of numerical data and easy manipulation of this data using NumPy. Thousands of datasets can be stored in a single file, categorized, and labelled as needed. h5py uses direct metaphors from NumPy and Python, such as dictionaries and NumPy array syntax.

File objects in h5py serve as the entry point into the world of HDF5. HDF5 files generally function similarly to standard Python file objects. In figure 2 is show the structure and content of an element of hdf5 file.

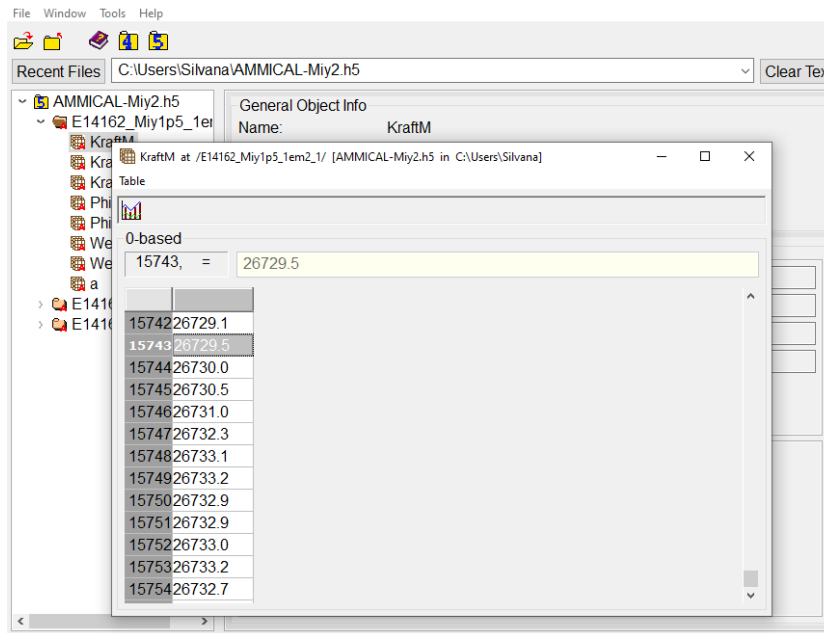


Fig 2: The structure and content of an hdf5 file

In the application, the method we used to interact with HDF5 files is `h5py.File('myfile.hdf5','r')`.

The web framework used for building this web application is Django. Django is a high-level Python web framework that encourages rapid development and clean, pragmatic design. The primary goal of Django is to simplify the creation of complex, database-driven websites. It provides an admin interface for easy management of the system, which makes it highly efficient for web development projects.

For the graphical representation of material data selected from the dataset, the Chart.js library has been utilized. Chart.js is a JavaScript library for creating charts that are based on HTML. It is one of the most popular libraries for data visualization in JavaScript, offering various types of charts, such as line charts, bar charts, pie charts, and more. Its simplicity, ease of integration, and wide community support make it a great choice for presenting material data in an interactive, visual format.

In combination, Django provides the backend framework, while Chart.js is employed on the frontend to present the data visually. The synergy between these two technologies ensures that the application not only handles complex data but also provides users with an intuitive, user-friendly interface for exploring and analyzing that data.

C. Application Architecture and its Structure

Django is based on the MVT (Model-View-Template) architecture. MVT is a software design model for developing web applications. The MVT structure consists of three main components as follows:

- **Model:** The Model acts as the interface to your data. It is responsible for storing the data. It represents the logical structure of the data throughout the entire application and is typically represented by a database, which is often a relational database such as MySQL or Postgres.
- **View:** The View is the user interface, what you see in the browser when you open a web page. It is represented by HTML/CSS/JavaScript files and Jinja (the template engine).
- **Template:** A template consists of static HTML parts and some special syntax that describes how dynamic content will be inserted as in figure 3.

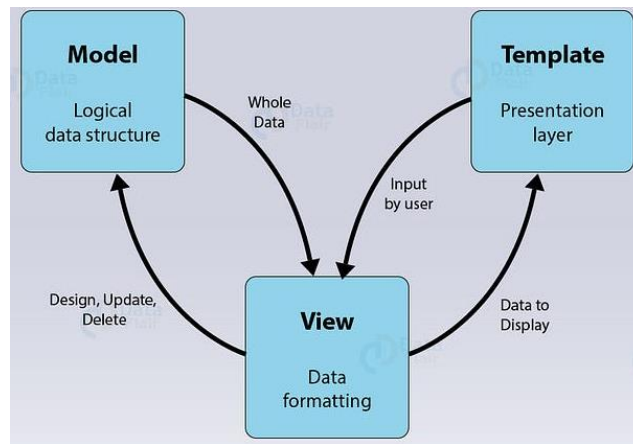


Fig 3: The architecture of Django [26]

A Django project, when initialized, contains basic files such as manage.py, views.py, etc. A simple project structure is enough to create an application with an interface, figure 4.

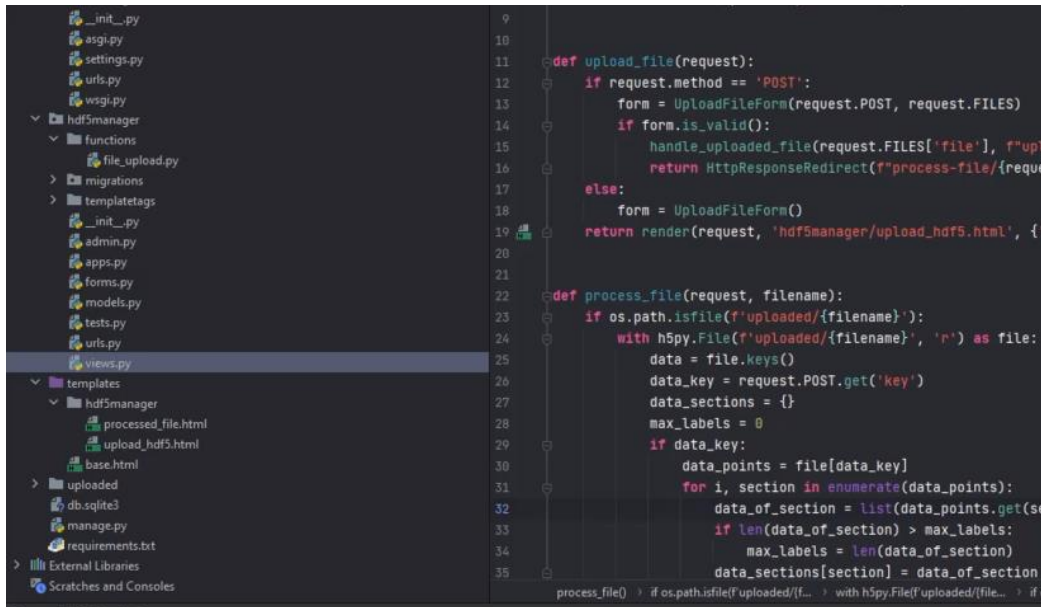


Fig 4: The architecture of the project in Django

manager.py – This file is used to interact with your project via terminal commands

__init__.py – It is a Python package. It is called when the package or a module in the package is imported.

settings.py – Contains all the settings of the application.

urls.py – This file holds all the URLs of the project and the functions to call.

wsgi.py – This file is used when deploying the project to WSGI.

models.py – A model is the single and final source of truth for data.

admin.py – Typically, this file contains models that we want to appear in the admin panel.

In the Uploaded folder, will be stored all the files that have been uploaded through the web interface of the application from the users. In the Template folder, there are the HTML files that will be rendered by the views, and they also contain Jinja syntax to populate the content dynamically.

D. Interface and Functionalities

The user interface is a key element when creating an application. The application has a simple interface and it is the only contact point that the user has with the application and through it accomplish a certain task. The application offers the ability to upload an HDF5 file with many records. Once the file the user

has selected it will be uploaded, the user will have the option to choose the dataset who wish to process, and then view its data in a 2D graphical representation, figure 5.

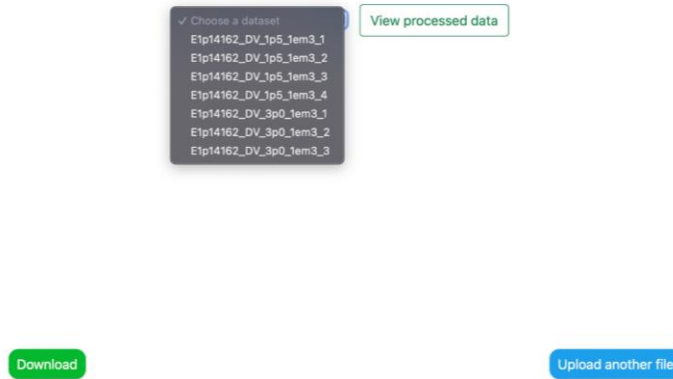


Fig 5: The datasets of the uploaded file

When the user clicks the button “View processed data”, the dataset will be display in a graphical form as in figure 6.

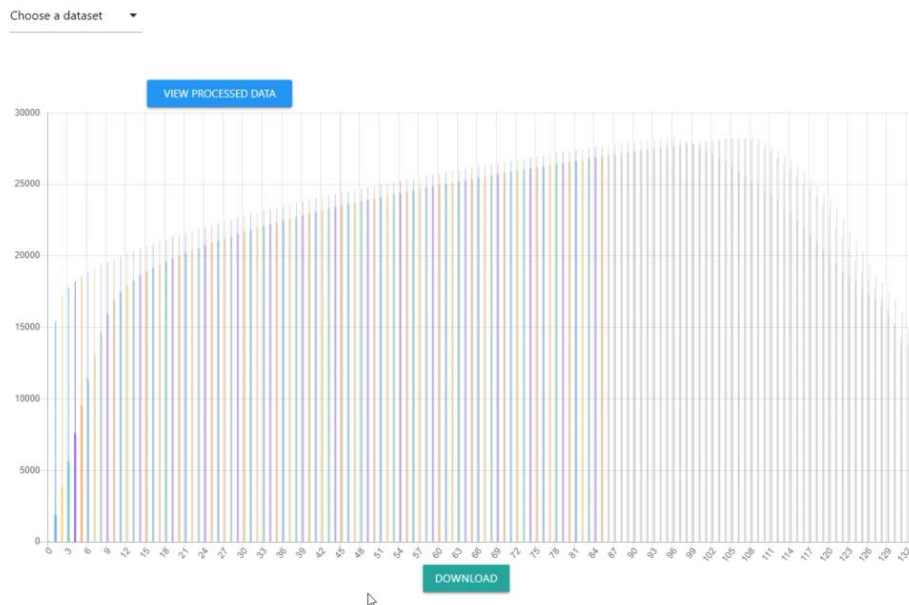


Fig 6: The graphical presentation of a dataset of hdf5 file

A graphical interpretation of another dataset of hdf5 file is given in figure 7.

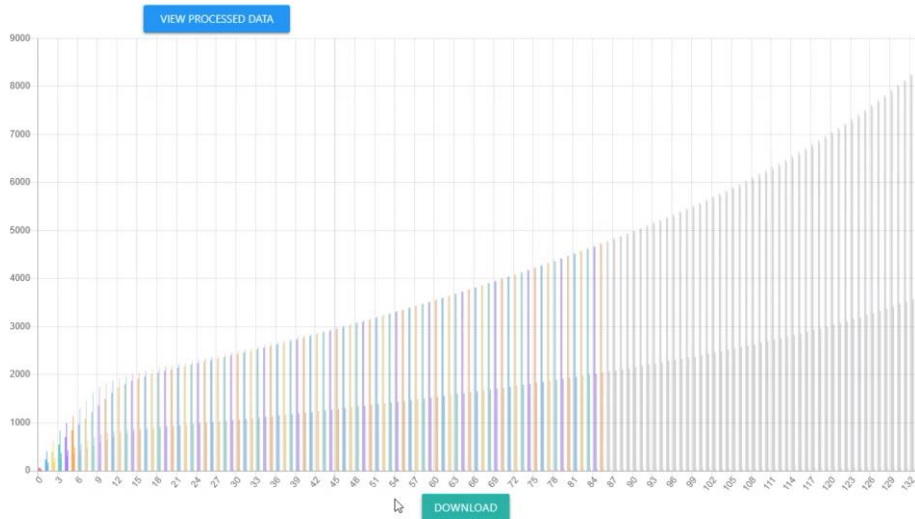


Fig 7: The graphical presentation of another dataset

The application also provides the option to download the graphical representation as shown above and allows the uploading of another hdf5 file. The user can download the graphic as an image and interpret it, figure 8.

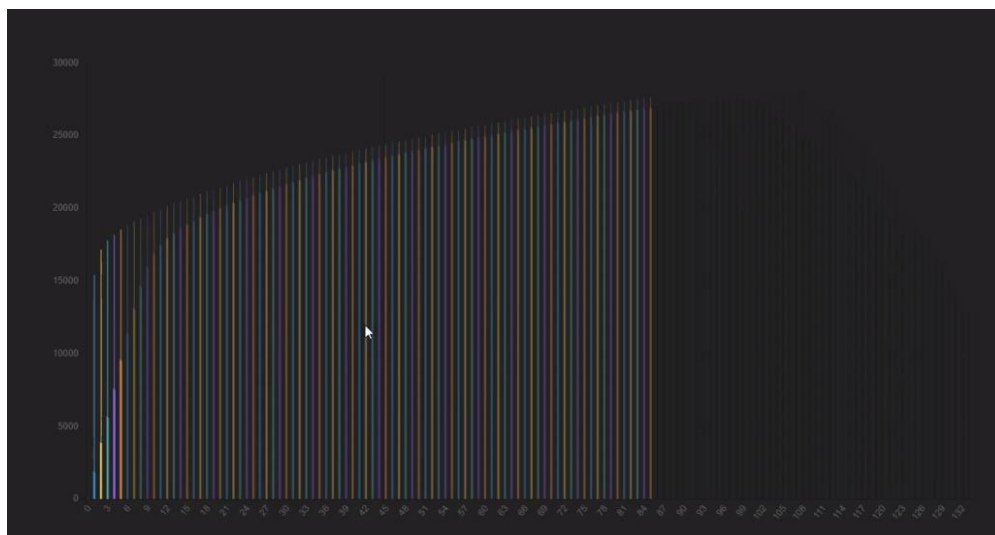


Fig 8: The image of the graphical presentation

In the admin panel, the admin has the ability to view all the HDF5 files that have been uploaded by the system users. All the uploaded files will be displayed, regardless of the user which has uploaded them as in figure 9.

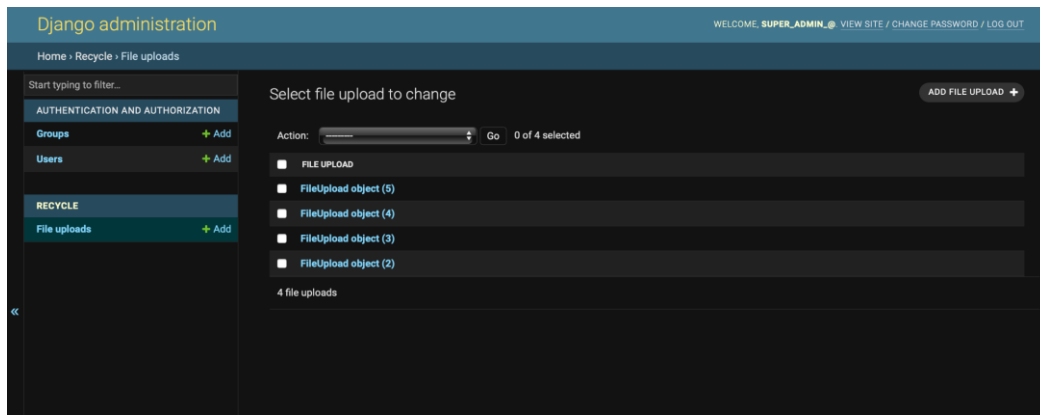


Fig 9: Admin view of uploaded file

VI. CONCLUSION

The aim of this paper was to review other academic and scientific works related to material data. A number of academic and scientific materials created by scholars worldwide were considered to reach all the results developed so far. The problems often encountered by workers and companies themselves are the lack of access to data for employees working in different locations around the world, which creates difficulties in performing comparative analyses, especially if the data they have is only from one part of the world or is not sufficiently linked to make accurate comparisons. The lack of automation in the process of recycling material data within companies that use this data slows down the workers' tasks and reduces productivity in the workplace. By automating this process, analysts could shorten the time needed to solve a problem, as they could determine how the findings from one data set could help answer another question more efficiently than would happen without this information. It would also improve collaboration, information exchange, and increase productivity in the workplace.

Digital recycling could enable any individual to overcome the risks of information overload and endless searches for information, which on a large scale in business can turn into macro threats to productivity.

Another point addressed in this paper is how well material data recycling is known in Albania and which Albanian companies have integrated this process. A survey was conducted with several questions, and the conclusion was reached that material data recycling is not well-known as a concept here in Albania, and those who had heard of it were not aware of any Albanian company using it. The automation of material data recycling would greatly assist workers in companies and increase productivity in the workplace.

The primary research of this paper, along with the conclusions drawn above, provides valuable findings for companies in various fields that use material data or even big data.

We have developed an application that read an old format such as HDF5. We find a simpler way to read an old file with material data and create a visual representation of it, aiming to reach a useful conclusion for people who use this data, such as engineers. The HDF5 format will be a file with multiple records for material data, ensuring the best performance using Python and Django.

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