

# Data Discovery and Indexing for Semi-Structured Scientific Data

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**Keywords:** Scientific Data Discovery, Data-Centric Indexing, Federated Data, User Interface, Semi-Structured Data.

**Abstract:** There is a need for powerful, user-friendly tools for scientific data management and discovery. We present an architecture based on DataFed and Elasticsearch that allows scientists to easily share data they produce and a novel interface that allows other scientists to easily discover data of interest. This interface supports summary-level information about a collection of datasets that can be easily refined using schema-free search. We extend the recent idea of cell-centric search to semi-structured data, describe the architecture of the system, present a use case from the context of materials science, and evaluate the efficacy of the system.

## 1 INTRODUCTION

Scientific experiments are time-consuming and costly. However, most data generated by researchers is stored in file systems where the only identifiable and searchable metadata is the file name and attributes. Funding agencies have expanded policies requiring scientific data to be made FAIR: Findable, Accessible, Interoperable, and Reproducible. However, many scientists view data management as a burden with questionable scientific value, as researchers have minimal tools to extract utility from their data. User adoption requires the combination of simplifying the burden and demonstrating added value.

When data is shared without tightly controlled schema, locating relevant data can be challenging because users do not know how the data is organized or what search terms to use. To solve this problem, we describe a solution based on cell-centric indexing (Heflin et al., 2021), which was initially devised for tabular data. In particular, we extend that paradigm to semi-structured data, such as JSON or multi-level dictionaries. JSON files encompass a multitude of nested key-value pairs, extending over multiple levels. Although key-value stores and graph databases are often suitable for storing JSON data, they require detailed knowledge of the structure to construct queries. This problem is exacerbated when many heterogeneous JSON files are stored.

To support data exploration by novel users, we propose building inverted indices using individual data items as the fundamental unit of semi-structured data. This approach, based on cell-centric indexing, enables flexible, schema-optional queries.

The contributions of this paper are: (1) We extend cell-centric indexing to the realm of semi-structured data, allowing users to discover and retrieve data without requiring prior knowledge of the specific keys and values within the semi-structured dataset. (2) We provide a comprehensive explanation of the system architecture. (3) We apply this approach to the domain of materials science. We also illustrate how a user-friendly interface design can effectively contribute to accomplishing the objective. (4) We assess the efficacy of indexing and querying datasets in terms of their efficiency.

## 2 BACKGROUND

Several projects present novel ways to search for specific datasets or to explore a collection of datasets. Chapman et al. (2020) provide a good review of dataset search while Maier et al. (2014) identify several challenges. Exploratory search requires interactivity and the ability of the user to filter the information (White and Roth, 2009). Some other examples

are He et al. (2008), Dunaiski et al. (2017) and Soto et al. (2015).

This paper is the evolution of research that began with a user-friendly exploration interface for distributed knowledge graphs (Zhang et al., 2013). That work combined tag clouds and faceted-browsing. Tag clouds are a popular visualization method that conveys data importance or frequency through varying font sizes. One inspiration for that work was Fan et al. (2009), who created an interactive user interface utilizing image clouds. Faceted browsing (Wongsuphasawat et al., 2016) is a ubiquitous paradigm found across the Web where users can filter the displayed information (e.g., a set of products in a store) by various categories (i.e., the facets). This interface lets users grasp their underlying query intentions and guides the system in curating personalized image suggestions.

These ideas were adapted to exploration for tabular data in developing cell-centric indexing (Heflin et al., 2021). The key idea is that individual cells of data tables are the key items of interest, and that indexing the properties of these cells enables schema-free search. The visualization allows the user to view summary histograms about the entire data collection; these histograms are organized by properties such as dataset title, column name, data value, and row context. Like faceted browsing, the histograms are recomputed as users specialize their queries, allowing patterns and anomalies to be discovered. To support the generation of the histograms, each cell is indexed in Elasticsearch using multiple fields. The underlying algorithms for computing the histograms rely on the notion of a conditional frequency vector (CFV) (Heflin et al., 2021). Each CFV summarizes the results of a query by providing a list of term/frequency pairs that describe the matches. This paper extends the concept of cell-centric indexing to semi-structured formats such as JSON, and applies the results to materials science as an exemplar.

Discovering new materials that underpin current and future technologies requires the ability to mine scientific databases. There has been work to organize this data via knowledge graphs and ontologies (McCusker et al., 2020), but such work requires data providers to “buy in” to the ontology. CRUX (Wang et al., 2022) is a crowd-sourced repository of materials science workflows but uses keyword-based search, requiring users to be familiar with the system’s ontology.

Materials science experiments often collect images via electron microscopy, but there is no common database for storing these images. One complication is that these experiments use collections of highly cus-

tomized systems that are rarely integrated or digitized.

### 3 DATA-CENTRIC INDEXING OF SEMI-STRUCTURED DATA

Semi-structured data is data that does not have a fixed schema, but instead schema information is embedded in the data. Typically, this data will have a tree structure. Thus, we can represent the data as a graph with two types of nodes: the complex nodes  $V_c$  and the atomic nodes  $V_a$ . Complex nodes are internal nodes, while atomic nodes are leaves that have values from a set  $D$ . Formally, the data is a graph  $G = (V, E, r, v)$  with nodes  $V = V_c \cup V_a$ , edges  $E$ , a root  $r \in V$ , and a function  $v: V_a \rightarrow D$  that assigns values to atomic nodes. Each edge is a tuple  $e \in V_c \times A \times V$ , where  $A$  is the set of attribute names. This general model can be used to describe the most common forms of semi-structured data: JSON and XML. For example, JSON consists of sequences of key-value pairs, where the values themselves can also be such sequences. In our abstract model, JSON keys are the attribute names, and each atomic value is associated with a node from  $V_a$ . We will consider each tree (typically one per file) to be a distinct dataset.

Compared to cell-centric indexing, the complex nodes provide schema information, while the atomic nodes contain data values. Thus, we need to index each node  $n \in V_a$ . A naïve approach would simply use the more specific attribute of each value when indexing, but this would lose all structural information conveyed by the nesting. Unlike tabular data, the schema information of  $V_a$  is not a column name, but instead the sequence of attribute labels for the path from the root  $r$  to  $n$ . One could concatenate this sequence to form a virtual schema entity, but there is no way to distinguish between a specific attribute label and its context. Another issue is that, unlike tabular data, there is no row; instead, a node can have siblings, and these siblings can have different attributes and values.

In the rest of the paper, we use the following functions as shorthand for referencing different parts of the tree: Given an edge  $e = (n_1, a, n_2)$ ,  $src(e) = n_1$  is the source of the edge,  $att(e) = a$  is the attribute of the edge, and  $dest(e) = n_2$  is the destination of the edge. Additionally,  $path(n)$  is the sequence of edges  $(e_1, e_2, \dots, e_k)$  along the path from the root  $r$  to node  $n$ ,  $out(n) = \{e \mid src(e) = n\}$  is the set of edges with  $n$  as a source,  $sib(n)$  is the set of nodes that share a parent with  $n$  (i.e., if the edge to  $n$  is  $(p, a, n)$ , then  $sib(n)$  is the set of all nodes  $n_i$  with an edge  $(p, a_i, n_i)$ ), and  $anc(n)$  is the set of nodes connected by the edges in

$path(n)$ , excluding  $n$  itself.

Like cell-centric indexing, each atomic node is indexed concerning several fields. These fields are summarized in Table 1. Note, the Type and Analyzer columns of the table will be explained in Section 4.2.1. The *value* field is the content of the atomic node  $n$ . The *attribute* field is the last attribute name on the path to  $n$ . The *pathname* is all other attribute names along this path. The *sibling\_context* is the set of values for all siblings of  $n$ . The *path\_context* is the set of values for all siblings of ancestors of  $n$ .

Algorithm 1 illustrates how to index a single node.  $IdxSS()$  is a recursive algorithm that performs a depth-first traversal of the tree. It is initially called with the root  $r$ , an empty string  $a$ , and empty sets  $path$  and  $pathcon$ . First, we collect all of the atomic node siblings in a set, and then collect all of the values of these sibling nodes (lines 2-3). If the current node  $n$  is an atomic node, then we index several fields with the appropriate values as determined by Table 1 (lines 4-9). The signature of  $Index$  is  $Index(field, doc, content)$ . We stress that a core idea of our approach is that the “document” is a data item, in this case, an atomic node  $n$  from the semi-structured document. Many values (i.e., those for fields *attribute*, *pathname*, *path\_context*) are provided as parameters as determined by the parent node. If the node is complex, we collect the outgoing *edges*, create a new  $path'$  by adding  $a$  to the set  $path$ , and create a new  $pathcon'$  by adding  $sibcon$  to  $pathcon$ . We then make a recursive call for each edge (lines 14- 15). Note, for brevity, we have excluded trivial elements of the algorithm, such as the indexing of the title field.

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Algorithm 1: How to index a node.

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1: procedure  $IdxSS(n, a, path, pathcon)$ 
2:    $sibs \leftarrow sib(n) \cap V_a$ 
3:    $sibcon \leftarrow \bigcup_i v(sibs_i)$ 
4:   if  $n \in V_a$  then
5:      $INDEX(value, n, v(n))$ 
6:      $INDEX(attribute, n, a)$ 
7:      $INDEX(pathname, n, path)$ 
8:      $INDEX(sibling\_context, n, sibcon)$ 
9:      $INDEX(path\_context, n, pathcon)$ 
10:  else
11:     $edges \leftarrow out(n)$ 
12:     $path' \leftarrow path \cup a$ 
13:     $pathcon' \leftarrow pathcon \cup sibcon$ 
14:    for  $e$  in  $edges$  do
15:       $IdxSS(dest(e), att(e), path', pathcon')$ 
16:    end for
17:  end if
18: end procedure

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## 4 SYSTEM ARCHITECTURE

There are three subsystems: Data Pre-Processing, Data Indexing and Retrieval, and a GUI for Data Discovery.

### 4.1 Data Pre-Processing

First, we upload relevant data in DataFed (Stansberry et al., 2019), a specialized platform designed for managing and organizing research data. DataFed provides a distributed scientific data management platform that is federated, scalable, and flexible for science, with elaborate administrative and access controls. DataFed repositories can be established at any institution but rely on a centrally managed metadata server. Metadata schemas can be designed using flexible JSON notation, and thus, DataFed is not restricted to specific scientific disciplines. Interaction with DataFed is possible through a command line interface, Python API, or a fully functional web interface.

Subsequently, JSON files are extracted from DataFed and processed according to Algorithm 1. The indexing calls are made to an Elasticsearch server, which is described in the next section. Domain-specific transformations can be applied here.

### 4.2 Data Indexing and Retrieval

The fundamental component of our system revolves around an Elasticsearch server, which serves as a scalable and distributed search engine with advanced analytical capabilities. The primary objectives of our system are: 1) Processing collections of datasets by extracting relevant information and organizing it into a set of data-centric fields. As field/value pairs are identified, they are sent to Elasticsearch through appropriate API calls. Elasticsearch builds the index, enabling efficient storage and retrieval. 2) Responding to user queries by executing a sequence of queries to Elasticsearch and generating specialized histograms called CFVs, for each field. These histograms provide a concise summary of the data distribution within each field.

#### 4.2.1 Indexing

It is common for search engines to create an inverted index for each of several fields, such as a *title* field and a *content* field. A query can target a specific field, or the document rankings might depend on which field a match occurred in. Fields can have different types and might be parsed into tokens differently. This information is provided by a mapping within the Elasticsearch framework. In our project, each data value

Table 1: Fields for indexing Semi-Structured Data.

Field	Definition	Type	Analyzer
value	$v(n)$	text numeric	whitespace_stop_analyzer NA
attribute	$att(e_k)$ where $path(n) = (e_1, e_2, \dots, e_k)$	text	wordDelimiter
pathname	$\{att(e_i) \mid path(n) = (e_1, e_2, \dots, e_k) \text{ and } 1 \leq i < e_k\}$	text	wordDelimiter
sibling_context	$\{v(s) \mid s \in sib(n)\}$	text	stop
path_context	$\{v(u) \mid a \in anc(n) \text{ and } u \in sib(a)\}$	text	stop
title	The name of the containing dataset	text	stop

serves as a document, and it is important that our index incorporates fields that accurately describe these data values. The last two columns of Table 1 describe the field type and the analyzer used to parse input.

We utilize three distinct field types: text, keyword, and double. Text fields undergo tokenization and are subject to word analyzers for processing. On the other hand, keyword fields are indexed in their original form without undergoing tokenization or additional processing steps.

Our system includes a few implementation-specific fields. While most of our fields are text fields, there are a few additional keyword fields: *fullTitle* allows users to access and view the complete name of the dataset in the search results and *datafedId* is used for provenance and to retrieve the raw data from DataFed.

It is important to note that we use two different fields to store different types of values: *value* and *valueNumeric*. The *valueNumeric* field is designated as a double field. This enables storing integer and real numeric values within this field. As discussed later, histograms with dynamically calculated buckets are created whenever numeric values appear in a query.

An analyzer is essential for properly handling text fields, as it determines the tokenization process and any additional processing requirements. In our system, we employ the stop analyzer for most text fields. This analyzer segments text by separating it at every non-letter character (e.g., whitespace, numbers, symbols, etc.) and eliminates 33 commonly occurring stop words, such as “a,” “the,” “to,” and others.

However, for the attribute and pathname fields, we utilize the wordDelimiter analyzer instead. This analyzer, in addition to separating text into special characters, also recognizes transitions in letter case. For instance, a term like “crystalStructure” would be tokenized into “crystal” and “structure”, taking into account the change in case. It is important to note that the wordDelimiter analyzer does not remove stop words from the analyzed text. For the *value* field, we used the whitespace\_stop\_analyzer, which is a variation of the stop analyzer that only considers whitespace as a token separator. Similar to the stop analyzer, it removes stop words from the text. However, it

does not separate strings that contain numbers or symbols. Thus, a chemical composition value like “Li V2 Cr1 O6” will be parsed into four tokens, “Li1,” “V2,” “Cr1,” and “O6,” instead of eight tokens, four of which are numbers.

#### 4.2.2 Handling Tensors

Scientific data often includes tensors, which are objects consisting of multi-dimensional numeric data. Given our emphasis on scientific data, we include special processing for tensors. In JSON, a tensor is encoded as a multi-dimensional array of numbers. Our interface (see Section 5) uses a distinctive notation:  $(\alpha)i, j$  to identify specific elements of relevant tensors. Here,  $\alpha$  stands for an unspecified tensor, while the *pathname* field can be used to determine the context of the tensor. However, the wordDelimiter analyzer is useful for most attribute names and will automatically separate numeric tokens from text strings. Therefore, our system must use an internal representation for the attribute name that does not include numbers or symbols. Our solution is to replace each number with a corresponding letter, resulting in a pattern “row” + *letter(i)* + “col” + *letter(j)* for a given tensor element. This results in attribute names such as **rowbcolc** to signify the positions of these values based on their row and column placements. When we display these tokens to users, we translate the codes into a more human-readable form. So, the code **rowbcolc** becomes  $(\alpha)2, 3$ , which makes it easier for users to see and understand how the different elements of relevant tensors relate to other data. When parsing semi-structured files, our algorithm assumes that any data that is a list of lists containing only numbers is a tensor, and assigns each element a field name as described above.

#### 4.2.3 Query Processor

The query processor takes user queries and generates CFVs that can be displayed as histograms. It submits textual aggregation requests to the Elasticsearch server and packages the response to provide search results to the GUI. The process details are described in Heflin et al. (2021).

When working with numeric data, histograms of distinct values are rarely useful. Unlike textual terms, numeric terms exhibit a greater variability. For example, “135”, “135.0” and “1.35E+2” are all equivalent, while some users might consider “135.0001” to be close enough. To address this, we create ranges over numeric values. Elasticsearch supports a histogram aggregation which can be used to build these distributions. However, a dynamic system for data exploration cannot predefine numeric ranges to serve as buckets for all possible data and queries. Our system dynamically creates buckets that are useful for any collection of numeric values that match the search criteria. The algorithm evaluated in this paper builds 5 buckets with sizes dictated by the distribution of the data. Once the numeric range CFV is created, this is merged with the token value CFV (Heflin et al., 2021).

### 4.3 GUI for Data Discovery

We have designed a GUI that enables users with the means to discover and interact with the data, even if they have no knowledge of the underlying schema. Specific interface examples can be found in Section 5.

Our interface is web-based, and thus based on HTML (Hypertext Markup Language) and CSS (Cascading Style Sheets). Interactivity is accomplished through a combination of JavaScript and TypeScript. We use Google Charts to generate and display histograms that convey information about the distribution of data that matches the user’s query through interactive visualizations.

## 5 INTERFACE DESIGN

We developed an easy-to-use interface that allows users to seamlessly navigate through the semi-structured data efficiently. Throughout this section, we will demonstrate the concepts for applications in materials science.

The Materials Project database<sup>1</sup> contains more than 150,000 materials whose structure and properties have been predicted using density functional theory (DFT) simulations. From the simulations, detailed information regarding the structural and functional properties can be obtained. Similarly, functional properties of materials, such as phonon structure, electronic structure, band gap, and magnetic properties, can be predicted. This resource can be used to discover materials with unique combinations

<sup>1</sup><https://next-gen.materialsproject.org/>

of properties. A common exploration might involve a multiparameter search that considers the chemistry, crystallographic structure, electrical conductivity, and piezoelectric tensor<sup>2</sup>. An exploratory search can expose specific chemistries, crystal structures, and associated properties that enable the achievement of application-specific figures of merit. Here, we use data-centric indexing of semistructured data scraped from the Materials Project and loaded into DataFed to demonstrate the discovery process of new functional materials.

The interface consists of seven interactive histograms, thus summarizing the data collection (or a subset of it) in a graphical form. Initially, two histograms, the Title Histogram and the Path Name histogram, are pre-loaded. These two histograms are most likely to define the context for the user’s search; to diversify the users’ choices, we also show twice as many values to serve as initial terms for the search. For example, our Title histogram will show that the Materials Project has data about different crystal symmetries, with Orthorhombic being the most represented, and Monoclinic the second-most represented. Likewise, the path name histogram, will contain attributes about symmetry, substrates, and structure, to name a few.

To observe the full set of histograms, the user must select a value from one of the initial histograms. For example, if the user clicks on *Hexagonal* in the Title histogram, that term is added to the query, and new histograms are generated to show what terms co-occur with it. The user can continue to refine the query by clicking on additional terms from any histogram. Figure 1 shows the path name, attribute, and value histograms after the user has additionally chosen the attribute “density”<sup>3</sup>. We can see that *piezoelectric* is the most common path name component found in datasets that match the query. As shown in the Attribute Histogram, these datasets have attribute names containing terms such as *density*, *atomic*, *ionic*, and *electronic*. These two histograms provide information about JSON keys in the indexed data. Users can click on any of these bars to refine their queries. To support expert users, the tool also has a feature where users can select an index field (such as those found in Table 1) and type in a query term.

Recall from Section 4.2.3, that our system dynamically create ranges for summarizing numeric values. These values are displayed as a range as

<sup>2</sup>Piezoelectric materials exhibit a linear coupling between the voltage and strain that can be used in energy conversion and sensing applications.

<sup>3</sup>Due to limited space, we do not show the other histograms.

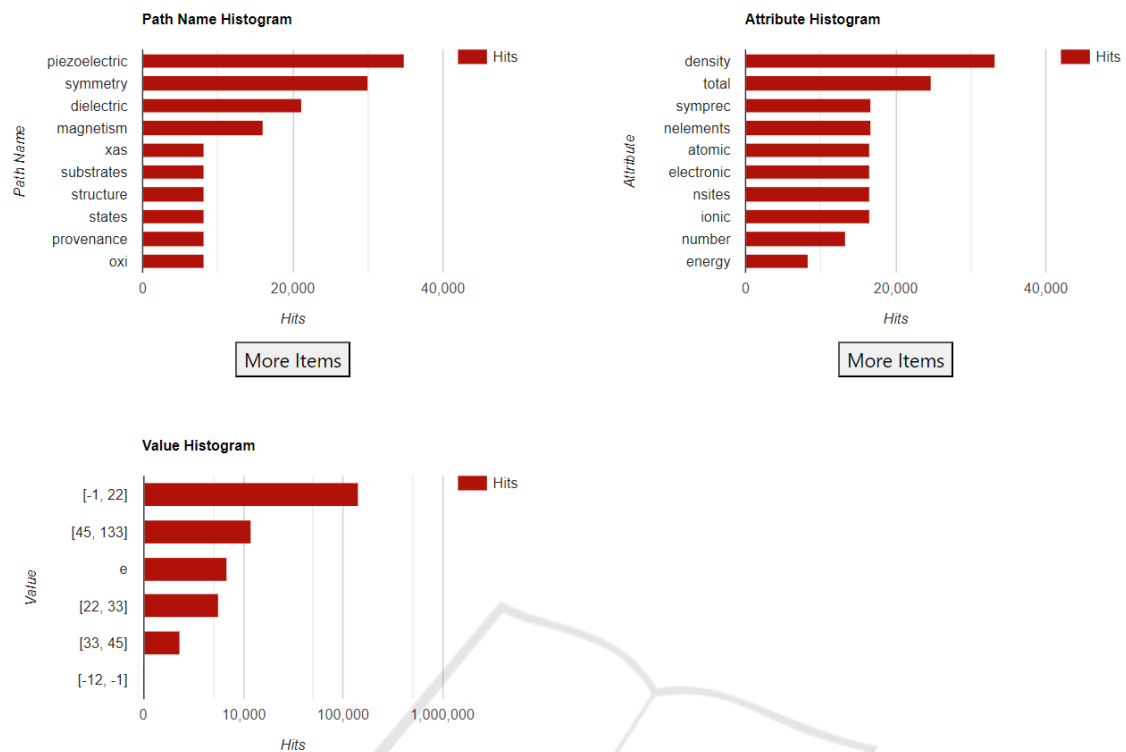


Figure 1: Path Name, Attribute, and Value Histograms after selecting title:“Hexagonal” and attribute:“density”.

[*lower\_bound, upper\_bound*]. Since the buckets aggregate values across all matching data items, they are not limited to values from any particular attribute/JSON key. Thus, by selecting a range of interest, the user will get context (such as path name, field name, and data set title) about where these data values are found. The Value histogram in Figure 1 shows several such ranges. We can see the count of these numerical ranges when we hover over the particular value. Additionally, clicking on a range will refine it by creating additional sub-buckets. One use of this is to look for outlier values and to identify patterns that lead to outliers. This feature is most useful after users have identified an attribute or path name of interest, but we emphasize that the generality of our system allows them to consider many different related attributes simultaneously.

As mentioned in Section 4.2.2, scientific data is often expressed as tensors. Our system automatically recognizes tensors and applies special indexing so that users can drill down to a particular element irrespective of the number of rows or columns. The fields for these values are prefixed with  $(\alpha)$ , representing a generic tensor, and any particular value can be accessed in the form of  $(\alpha)_{row, column}$ . For example, if we have 3 rows and 4 columns, there will be 12 distinct entries in the attribute histogram. The

entry for the third row and second column will be referenced as  $(\alpha)_{3, 2}$ .

When the user clicks any tensor element, based on the previously described process of numerical buckets, the values of these tensors are automatically bucketed. Alternatively, a user could select a value range, and see which tensor elements have values in that range.

With each query, a full title histogram is constructed and displayed at the bottom of the screen. This summarizes which datasets/files contain the most values matching the user’s query. Hovering on the bars of these histograms displays additional data like the DataFed id, etc.

Finally, once we identify the particular file we are interested in, to further explore it in its original form, its corresponding JSON file is retrieved from DataFed and is displayed using a JSON viewer in a separate tab by passing the corresponding DataFed id as the input parameter.

## 6 PERFORMANCE EVALUATION

We conducted experiments to evaluate the system’s performance in terms of indexing scalability and query execution time. The experiments primarily fo-

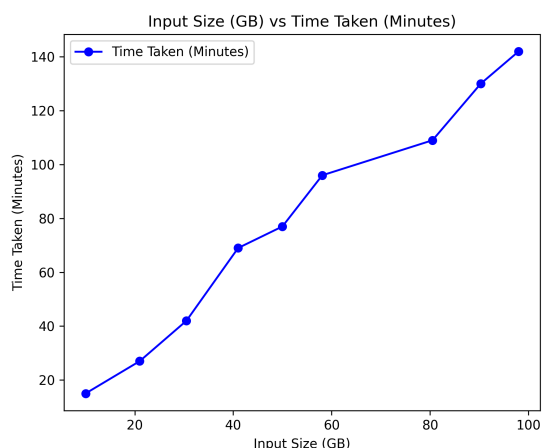


Figure 2: Time to index for different sizes of inputs.

cused on utilizing data from the Materials Project, comprising a collection of 10,000 semi-structured JSON files. Characterized by the properties of trees, these files have an average depth of 4 and a maximum branching factor of 77 (at the first level). All of our experiments are conducted using a Lehigh-hosted server. The server has one Intel(R) Xeon(R) Silver 4110 CPU @ 2.10GHz, with 8 cores (16 threads) and a total of 96GB RAM. It runs Java 11.0.7 and Elasticsearch 6.8.8.

The entire collection of files was loaded in batches, with each subsequent batch increasing in size. The indexing process was conducted for different percentages (20%, 40%, 60%, 80%, and 100%) of the 10,000 semi-structured JSON files comprising nearly 100GB of data. Overall, there exists a linear relationship between size and load time, as shown in Figure 2. It took 143 minutes to index the entire collection.

Indexing individual data items can use significant disk space. Therefore, we also measured the size of the resulting index in proportion to the original JSON files. Again, the relationship is essentially linear (not shown due to space limitations). On average, the indexed file is  $\approx 36\%$  of the input size. We note, however, that this relationship depends heavily on the structure and content of the indexed files.

To measure query execution time, we had to generate a workload of realistic test queries. Note that simply choosing a set of random query terms will often lead to queries with no results. Such queries are usually executed quickly and will lead to an overly optimistic evaluation. Given that our system uses incremental query construction, it is also important that the queries follow plausible paths. Hence, we generated queries utilizing the available materials science data. The queries were formulated in five distinct steps, starting with a single query search term (con-

Table 2: Query Execution Time as Query Length Increases.

Search Terms (#)	Time (sec)
1	1.19
2	1.48
3	0.40
4	0.23
5	0.29

sisting of a pair of fields and terms) in the first step, followed by adding a second query search term in the second step, and so forth, until reaching the fifth step with five query search terms. Since our interface restricts the initial query to terms from the title histogram and path name histogram, our query generation places a similar restriction on the first step. Subsequently, the second, third, fourth, and fifth queries, as outlined, will be derived from the subset of data that already satisfies the condition established by the first selected search term. This is done to ensure non-null results. In each combination, a total of 10,000 queries were generated, resulting in an aggregate of 50,000 queries that were generated to capture and analyze query execution time.

To evaluate query execution time, we executed these 50,000 queries on the full index of 10,000 files ( $\sim 18$ GB in size). The average query times, grouped by the number of search terms, are shown in Table 2. Generally, query time decreases as the number of search terms increases. Since the query is conjunctive, adding more terms makes it more selective, and the system can create histograms over fewer results more quickly. Although the average for one and two search terms was above 1 second, only 0.0015% of all queries took 1 second or more. This means there were a few outliers that impacted the average. Upon investigating the reasons for the outlier queries, it was observed that the increase in time is directly proportional to the count of matched cells in our database. In particular, there was an increase of 85% in matched cell count that resulted in the increase of time by 82%. This occurred for a few very common query terms, especially for widespread crystal systems such as “Orthogonal”. Usually, such queries like crystal systems will be part of the broader filter and hence end up being in first or second query search terms. Hence, the average query time for one search term and two search terms is approximately 3.5x more compared to the remaining search terms. One possible solution to handle such outlier queries is to use a caching mechanism for such popular queries.

## 7 CONCLUSION

In this paper, we present a novel approach to exploring collections of semi-structured data by extending the cell-centric indexing approach. We emphasize the importance of a user-friendly interface in achieving the overarching objective of data exploration and retrieval tasks. Our solution takes about just over an hour to index 40 GB of semi-structured data. Over 99% of the queries are executed in under one second. Our work not only empowers researchers to effortlessly access and retrieve data without prior knowledge of its organization but also highlights its applicability in material science.

Our short-term plans include incorporating our system into the experimental pipeline of a small number of materials scientists. We will collect feedback via surveys and think-aloud studies, adjust the system as necessary, and expand the user group. A key step is explicitly incorporating images, especially microscopy. Recently, Nguyen et al. (2021) demonstrated the capabilities of a symmetry-aware neural network featurization in exploring large unstructured databases of microscopy images. We intend to explore ways to use image embeddings as additional criteria for refining searches, while maintaining the performance we achieved by using Elasticsearch as our backend indexing system. By integrating database management, ontology development, and machine learning, we aim to enable efficient metadata searches and facilitate the comparison of physics-aware features within microscopy images. This initiative holds the promise of accelerating the exploration of synthesis-structure-property relationships to advance materials design. Although our emphasis has been on scientific data management, these approaches are general enough to be applied to any enterprise that has a data lake of semi-structured data.

## ACKNOWLEDGEMENTS

This material is based upon work supported by the National Science Foundation under Grant No. 2246463

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