DaedalusData: Exploration, Knowledge Externalization and Labeling of Particles in Medical Manufacturing – A Design Study – Supplemental Materials

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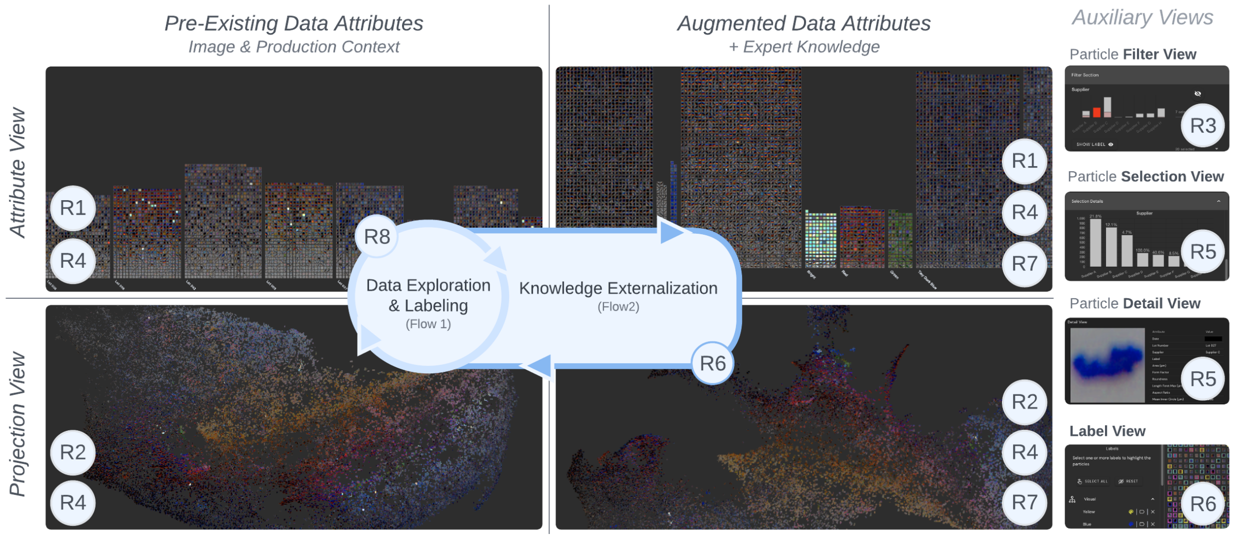

Fig. S1: DaedalusData enables experts to explore large numbers of particle data, and externalize knowledge through enhanced interactive labeling. In the DaedalusData framework, experts have two main types control to steer the particle display, conceptualized in a 2×2 matrix, the cross-cut leads to four unique recipes to display particle images on the main canvas. Vertical: experts decide between a single-attribute (Attribute View) and a user-selected multi-attribute display (Projection View). Horizontal: experts choose to explore pre-existing attributes (here: Image & Production Context), or extend the exploration to augmented data attributes created through particle labeling (Expert Knowledge). In this design study, our solution implements the systematic cross-cut of all four types of control, addressing crucial requirements gathered with experts. DaedalusData enables experts to conduct two dominating workflows: Data Exploration and Labeling (Flow 1), and its extension, Knowledge Externalization (Flow 2). On the right, we introduce four auxiliary views, necessary for experts to facilitate interactive drill-downs, particle selection, detailed analysis, and perform labeling.

Abstract—These are the supplemental materials for DaedalusData: Exploration, Knowledge Externalization and Labeling of Particles in Medical Manufacturing – A Design Study. Here, we provide supporting information on data preprocessing, our executed User Study, the DaedalusData's evolution through our design iterations with detailed views of the process, and the DaedalusData software architecture.

Index Terms—Visual Analytics, Image Data, Knowledge Externalization, Data Labeling, Anomaly Detection, Medical Manufacturing

S1 Preprocessing Pipeline

- **Resizing and Padding:** Images are resized to a standard dimension while maintaining their aspect ratio. Padding is applied to ensure that all images have the same shape, which is necessary for batch processing in machine learning models.
- **Color Normalization:** The Reinhard color normalization method is applied to standardize the color distribution across different images, which helps in reducing the variability due to lighting conditions and enhances the model's ability to learn relevant features.
- **Background Segmentation:** Images are processed to identify and extract the largest connected component, which typically corresponds to the particle of interest. This step reduces the influence of background noise and focuses the analysis on the particle itself.
- **Rotation and Alignment:** The extracted particle is then aligned such that its longest dimension is horizontal, which standardizes the orientation of particles across the dataset and improves the consistency of feature extraction.
- **Feature Embedding:** Finally, the preprocessed images are fed into a pre-trained convolutional neural network (CNN), EfficientNetB0 in this case, to extract high-level features. These features serve as a compact representation of the images and capture complex patterns that are difficult to quantify with traditional image processing techniques.

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S2 User Study Agenda

Below is the guide we used when evaluating the tool with participants from **Roche Diagnostics**.

S2.1 Greeting and explanation of the Setup

1. "Welcome to the study and thanks for participating. . . "
2. "I will record this user study is it ok if I start the recording?" start recording
   - Do not mention that I will label the facial expressions from the video (TMI)
3. "In this user study, you will be asked to evaluate the tool DaedalusData, which was developed as part of my master thesis. The tool was built to analyze particle contaminations in our products. historically, we performed cleanliness analysis and evaluated them mainly based on how many and how large the particles were. With this tool, we want to inspect what particles are found by looking at their metadata and visual similarity. Plainly spoken, we want to find out if there are for example distinctly green or very bright, reflective particles in those inspections. This could help us to investigate where it is coming from and evaluating if we can do something to counteract this."
4. "DaedalusData will display many particle images and group similar particles together. To give you a better impression of how the tool works you can watch this short tutorial video which shows you the main functionality of the tool. You will be able to replay this video if you want during the study, or also ask questions if anything is unclear." Play Video
5. "Now that you have watched the video please take 2–3 minutes to get familiar with the tool, make sure to cover the following points"
6. "Please keep in mind that you are not tested, but the tool is" make sure that the user performs at least the following tasks
   - Move around on the screen by holding and dragging the left mouse button
   - Zoom in and out of areas which interest you using the mouse wheel
   - Click on one Particle using a left mouse click to view its details
   - Select multiple particles with the lasso tool, hold and drag with a right mouse click
   - Create multiple lasso selections by holding CTRL
   - Clear the selection by pressing ESC
   - Switch to the transparent representation of the particles in order to filter out the background
   - Deselect selected or select unselected particles by holding CTRL + left mouse click on individual particles
   - Switch to a new Attribute View
   - Switch to a new Projection View
7. "Next we will start with some tasks. I will give you three tasks one after another, which I want you to perform. Please feel free to experiment with the tool and think aloud during your process and describe what you are thinking."

S2.2 Task Execution (Approximately 10-30 minutes)

S2.2.1 Task 1: Data Exploration (3-5 minutes)

- "We have had a field-complaint that a green substance was found in one of our products produced by Supplier 1. Unfortunately, we did not get any further details. Can you identify all particles that match this rough description"
- Instruct the participant to identify a specific group or area of interest within the dataset. Ask them to explain their criteria for choosing this group. Guide them to utilize the zoom functionality (mouse-wheel zoom and representation resizing) to better examine their chosen area. Ask the participant to apply metadata and label-based filtering to their chosen group or area. Encourage the participant to click on an individual image or use the lasso tool to select a group of images within their chosen area to view details on demand.
- Solicit their feedback on the efficiency and intuitiveness of these functionalities.

Acceptance Criteria:

- Participant found any green particles
- Participant found at least one larger group of green particles
- Participant found multiple groups of green particles

S2.2.2 Task 2: Data Labeling (3-5 minutes)

- "Please add a appropriate label to the green substance particles you found before"
  (27 min first label assigned)
- "Continue on your own to label two or more groups, you can either add more particles to an existing label or add a completely new one"
- "The Labels aren't jet assigned to a label alphabet, let's add one for the new labels" Guide user if he does not find it after some seconds
- Instruct the participant to assign a label to their selection. They can choose from existing labels or create a new one.
- Request them to review their labeling and make adjustments if necessary.
- Encourage them to share their thoughts on the ease and efficiency of these processes.

Acceptance Criteria:

- Participant was able to assign an appropriate label name at least two green particles.
- Participant was able, after labeling to inspect the selection details for the labeled particles.

S2.2.3 Task 3: Knowledge Externalization (3-5 minutes)

- Guide the participant to navigate through a label-informed projections.
- Make sure to cover:
  - at least one Attribute View
  - at least one Projection View, which the user updates
  - at least one label-informed Projection View
- Each projection represents dimensionality reductions created using different attributes or parameters. Ask them to share their observations and compare the projections.
- Ask the participant how comfortably they can navigate through these various projections.
- Request them to discuss any difficulties they faced and share their suggestions to improve this feature.
- Throughout the task execution phase, remind the participant to think aloud and share their thought process and experiences as they navigate and interact with the tool. This will provide you with real-time feedback and valuable insights into user interaction with your tool.

Acceptance Criteria:

- Participant was able to navigate to each Attribute/Projection View
- Participant mentioned for at least two different views that they were insightful

S2.2.4 Post-Task Evaluation

At the conclusion of the tasks, we will perform a post-task evaluation using the NASA Task Load Index (NASA-TLX) [3]. The NASA-TLX is a well-established tool to assess perceived workload and cognitive load.

- "Now that we have completed the tasks, we're going to shift gears a bit. We will be conducting a brief evaluation using the NASA Task Load Index, a tool that will help me understand how you perceived the workload of the tasks you just performed."
- "I'll be showing you a series of pairs of words, such as "Mental Demand" versus "Physical Demand," and asking you to mark on a line where you think the tasks fall. Please keep in mind, there are no right or wrong answers. We're interested in your personal experience."

- “Afterward, you’ll rate the degree of each factor (e.g., effort, frustration) in the tasks you performed on a scale of Very Low to Very High. It’s important to give each question careful consideration, but don’t overthink your answers. Your initial gut response is usually the best one.”

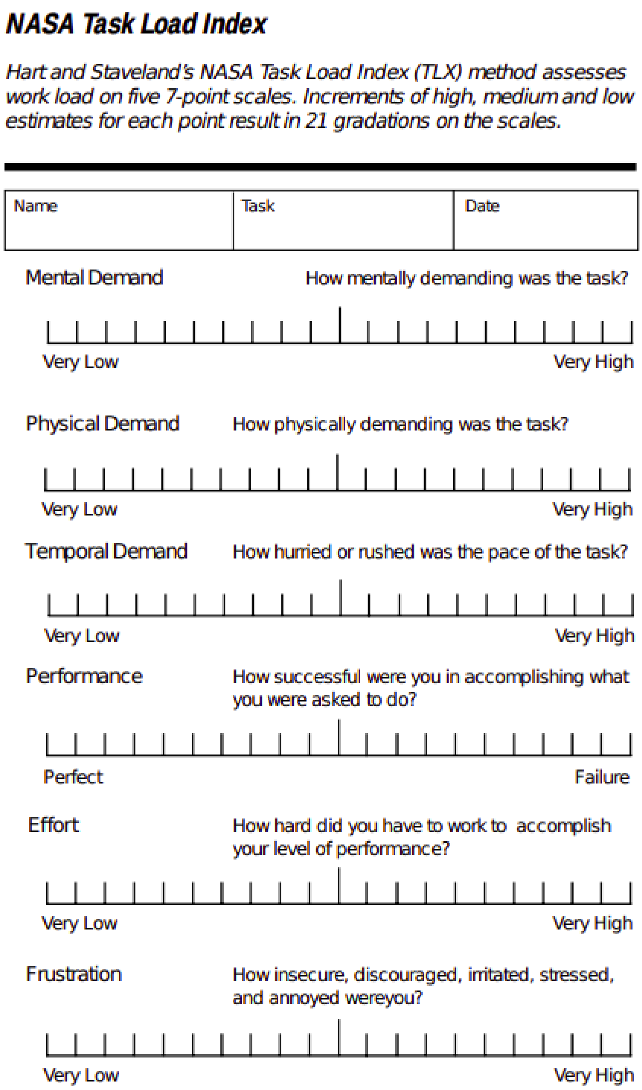


Fig. S2: The NASA TLX survey tool, as applied to participants in our user study evaluation.

S2.2.5 General Debriefing and Open Feedback

- “Thank you for completing the NASA TLX evaluation. We are now moving to the last stage of our user study - the general debriefing. This is a chance for you to freely share your thoughts and feedback.”
- “Overall, how was your experience with the tool?”
- “What did you like most about the tool?”
- “Was there anything you found particularly difficult or frustrating?”
- “Were there any tasks that you felt could have been performed more efficiently?”
- “Do you have any suggestions for features or improvements that could enhance your experience with the tool?”
- “Thank you again for your time and insights today. Your feedback is extremely valuable and will play a crucial role in improving the tool. Your contribution is greatly appreciated.”

S3 DaedalusData’s Design Evolution

This subsection presents our iterative development process, and its narrative showcases the evolution of DaedalusData’s design, usability, and usefulness. Each figure represents a milestone in the design process, reflecting the emphasis we placed on listening to expert feedback in the development of this tool.

Figure S3 shows the first sketches that took place shortly after initial discussions with E1, M1, and M2. The Figma sketch in Figure S4, created later in the same cycle, explored different approaches for how to highlight elements on the Canvas. Most of the initial designs centered around a central Canvas, projecting particle images on it. This is a design concept our collaborators connected with early in the tool’s development. Based on this concept, additional component sketches were drawn (Figure S5a). Figure S7 shows the first version that shared usage concepts with the current version of DaedalusData.

The initial cycle also included ideation on possible technology stacks. A first version interactive version of the tool, was created, using Vue.js as a frontend framework and D3.js [1] for the Canvas visualization. As legal contracts were still being negotiated, we started working with masked and test data, hence the censored portion of Figure S6. The central Canvas, showing the particle images, is now built with Three.js [2] on a Vue.js frontend.

In the second development cycle, we implemented the first selection tool, seen in Figure S8, and S9. This allowed for single-particle selection using a rectangular tool, and for experts obtain summary statistics on the attributes of their selection. This cycle also introduced the first Attribute View (Figure S10), allowing for a simple and fast comparison of suppliers. Note how the sidebar navigation already resembles the current version of DaedalusData.

The third cycle introduced a dark mode, which improved the ability to identify visual patterns significantly (Figure S12 and Figure S11). We also experimented with an extended Particle Selection View (Figure S12), including Canvas interactions allowing for dynamic grouping and inspection of user defined attributes, using bar charts and letter-value plots. We ultimately decided against this version of the Particle Selection View, as it did not scale well to the amount of data we analyzed. However, this version received very positive feedback from informal discussions with experts.

In the fourth and last cycle, seen in Figure S13, most of the remaining functionality was added to the tool. At this stage, we refined Canvas-based navigation, and combined the selection, selection details, and labeling of particles into same Auxiliary View. A final version of our Labeling Auxiliary View can be seen in Figure S14. Our final implementation was created according to the architecture described by Figures S15 and S16.

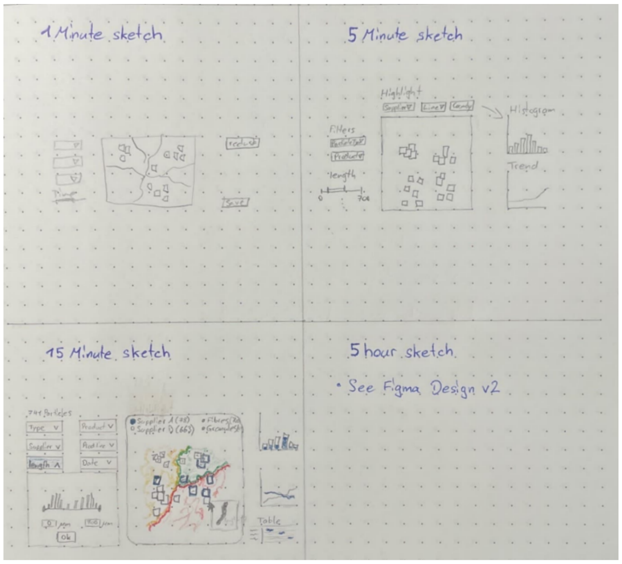
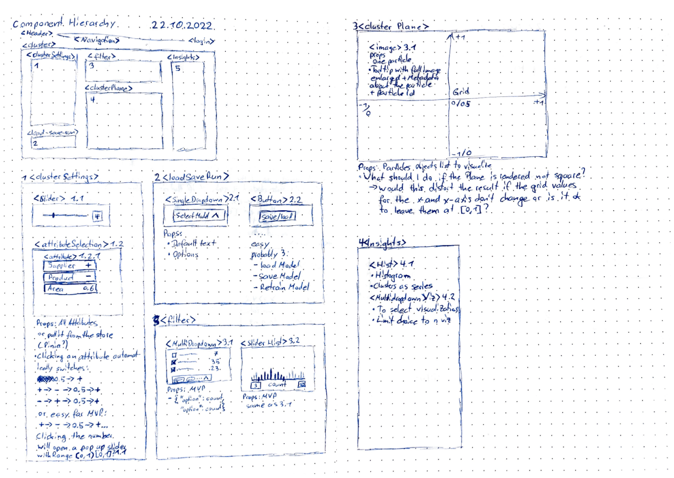


Fig. S3: Initial paper sketch outlining the basic layout and interaction concepts.

Fig. S4: Digital sketch created in Figma, refining the initial concepts and exploring color schemes for particle groupings.



(a) Initial sketch of UI component 1

(b) Initial sketch of UI component 2

Fig. S5: Initial sketches for UI elements and their layout

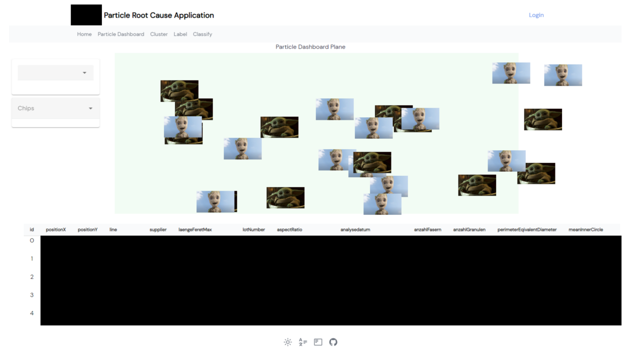


Fig. S6: First programmed and interactive version of the tool, using test data and including a table of item attribute values at the bottom (censored).

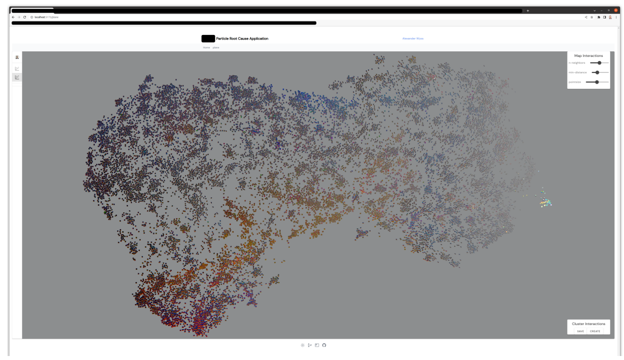


Fig. S7: Early version of the UI showing a simple plane projection of the data (V 1.3.0).

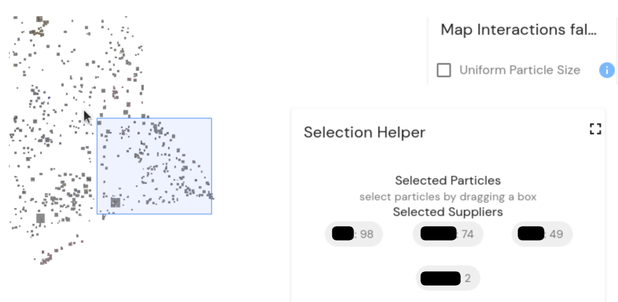


Fig. S8: Updated UI with a navigation sidebar already on the left and plane in the center (V 1.6.0).

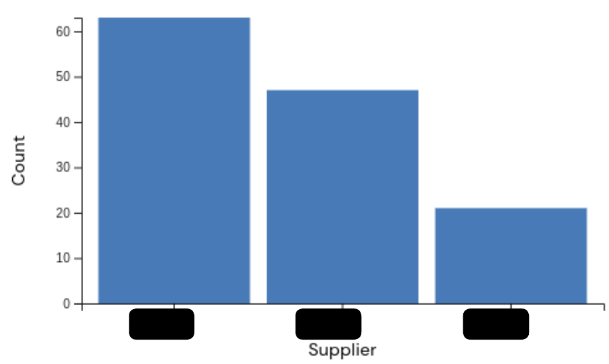


Fig. S9: Integration of a bar chart for attribute distribution, facilitating data analysis (V 1.6.0).

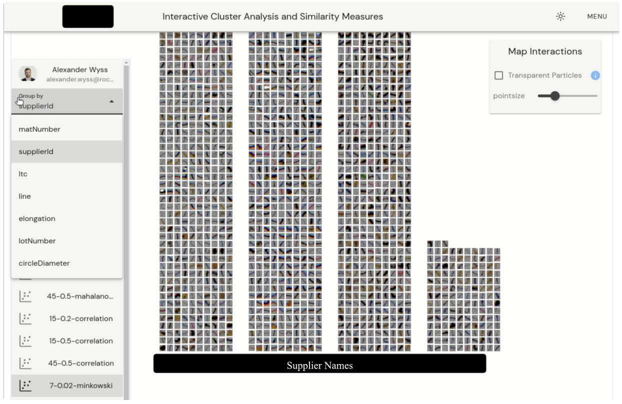


Fig. S10: Introduction of attribute projections, allowing experts to explore data based on specific attributes (V 1.7.0).

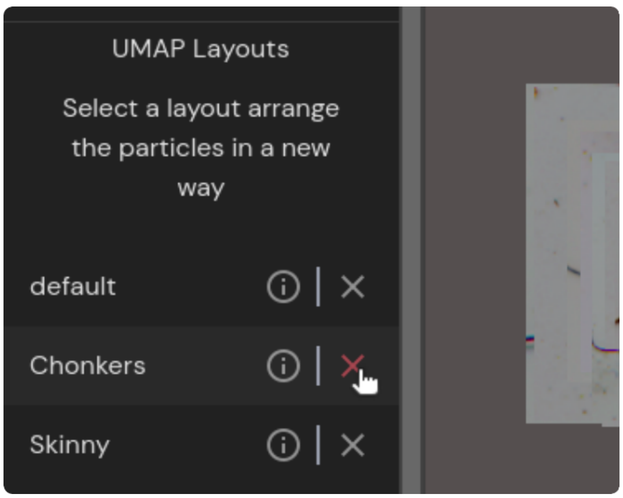


Fig. S11: Similarity projections feature, enabling experts create or manage dimensionality reduced projections calculated on their data selections (V 1.8.0).

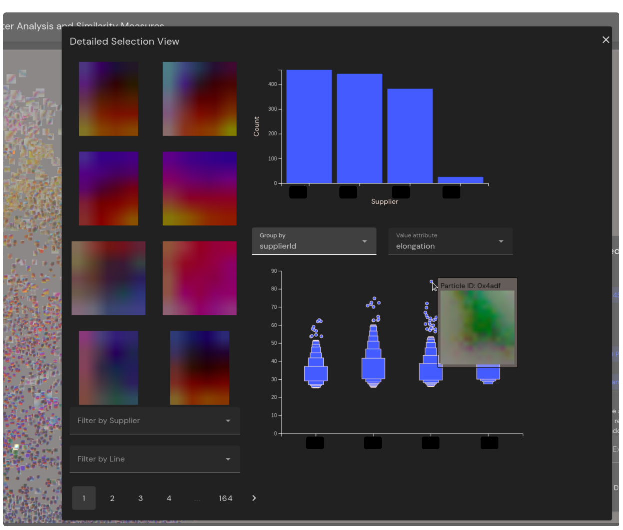


Fig. S12: Extended selection details with letter value plot, providing in-depth analysis of selected data. This view was considered insightful by experts, but some aspects did not scale well to the number of particles we had in scope (V 1.8.0).

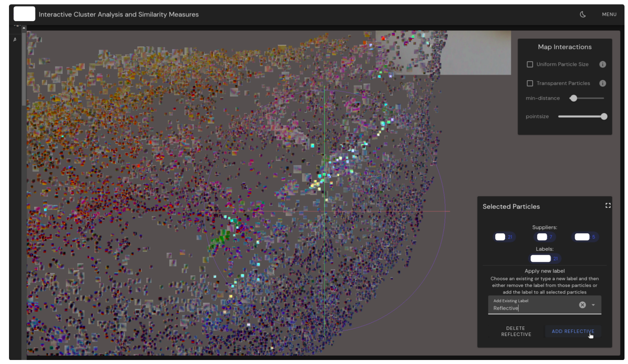


Fig. S13: One of the final UI iteration with refined plane projection and streamlined user interactions (V 1.9.0).

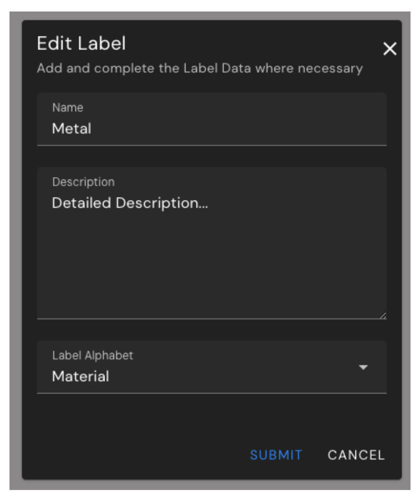


Fig. S14: The Label View, where an expert edits a label to include a meaningful name and (optional) description of the associated particles. They can also add this label to a label alphabet, further externalizing knowledge gained from data exploration.

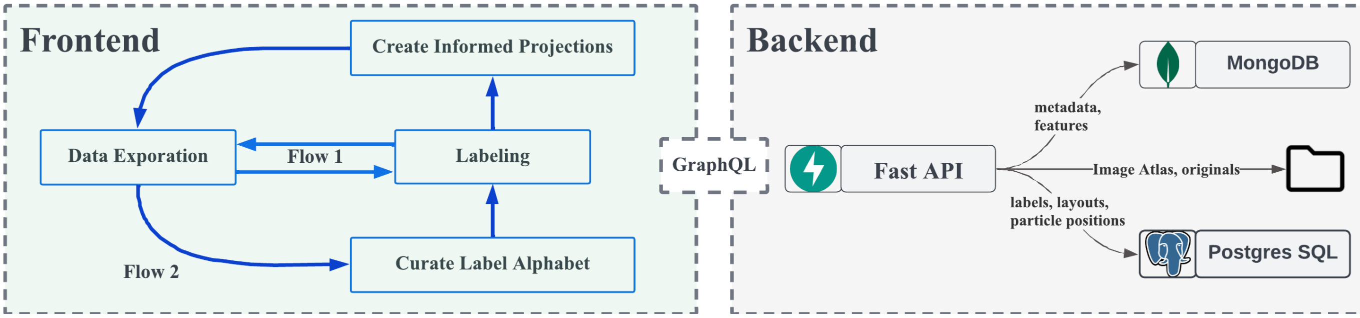


Fig. S15: An overview of the responsibilities of each backend software DaedalusData leverages, as well as the frontend workflows this architecture supports

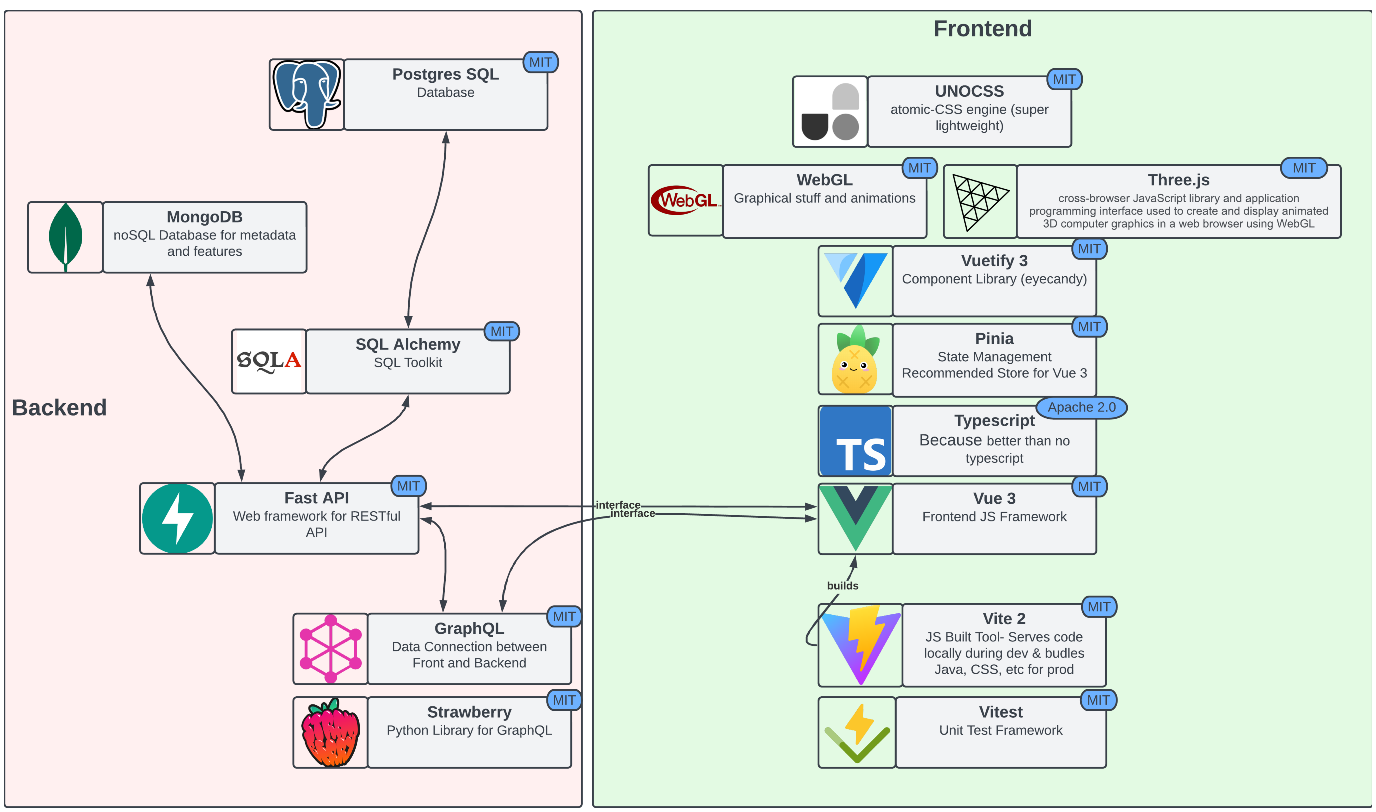


Fig. S16: A detailed view of the final architecture of DaedalusData, including all frontend and backend software leveraged and its purpose in the implementation

S4 Tool Performance

As a research prototype DaedalusData was deployed locally at the time of the user and case studies. This includes the backend as well as the frontend. The following number shall provide a better overview of the performance of DaedalusData, on relatively low-powered hardware.

Hardware: Apple MacBook Air M1, Memory 16GB **Number of Particles:** 37'857

- Initial fetch - 17s

  On startup, the dataset is loaded into the browser, this includes the complete metadata of the tool, as much of the computation is performed client side as of then
- Loading a new projection - 4.5s
- Loading a previously viewed projection - <1s
- Training/Re-training a projection - 37s

  Utilizing all, image, attribute and labels as features and target vectors for UMAP

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