

User Guide: CrysAI TM Offline Particle Characterization App

Prepared by APC Innovation Team
Built with Python Shiny & Detectron2

1. Introduction

CrysAI TM is an interactive web application for analyzing images of crystals for particle shape and size characterization. Powered by deep learning-based image analysis (**DLIA**), the app segments crystal particles and calculates critical morphological descriptors including length, width, aspect ratio, circularity, roughness etc., and their distributions (D10, D50, D90).

2. Key Features

CrysAI TM allows users to *Upload Images* from different acquisition tools i.e. SEM, optical microscope, PVM, Easyviewer etc., for offline analysis of crystallization particles morphology. Once uploaded, the images are automatically processed using a deep learning-based segmentation model, which performs instance segmentation to detect and isolate individual particles within each image.

Following segmentation, the app extracts key morphological metrics such as particle length, width, area, aspect ratio, and circularity. Users can visualize results through overlay images with segmentation masks, interactive metric tables, and distribution plots. All processed data, including numerical results and visual outputs, can be downloaded for further review or documentation. Figure 1 is a brief overview of the application workflow.

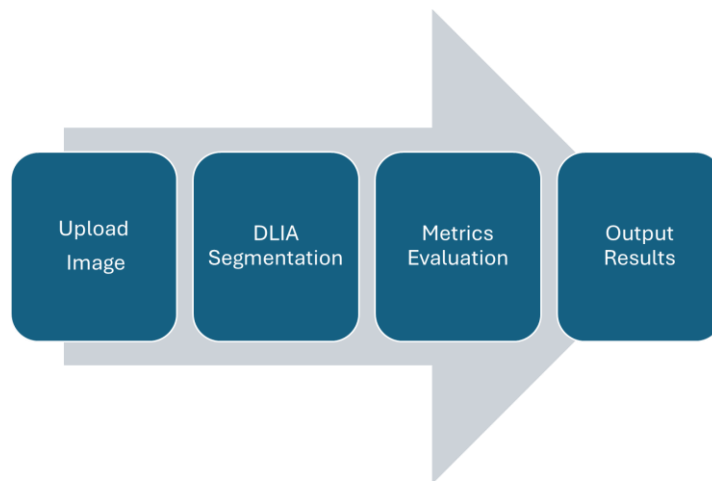


Figure 1 | Overview of App Workflow (Input → Segmentation → Metrics → Output)

3. Getting Started

3.1 Launching the App

Open the app from the iAchieve Virtual Experiment (VE) Tab or the TME Web App store on your browser. Depending on deployment, you might access it through a URL link or application shortcut. [App Link: www.apcinnovate.shinyapps.io/dlia_offline_particle_characterization]

Figure 2 shows the login page of the application, prompting users to enter a supplied username and password to access the App after opening the linking in your preferred browser.

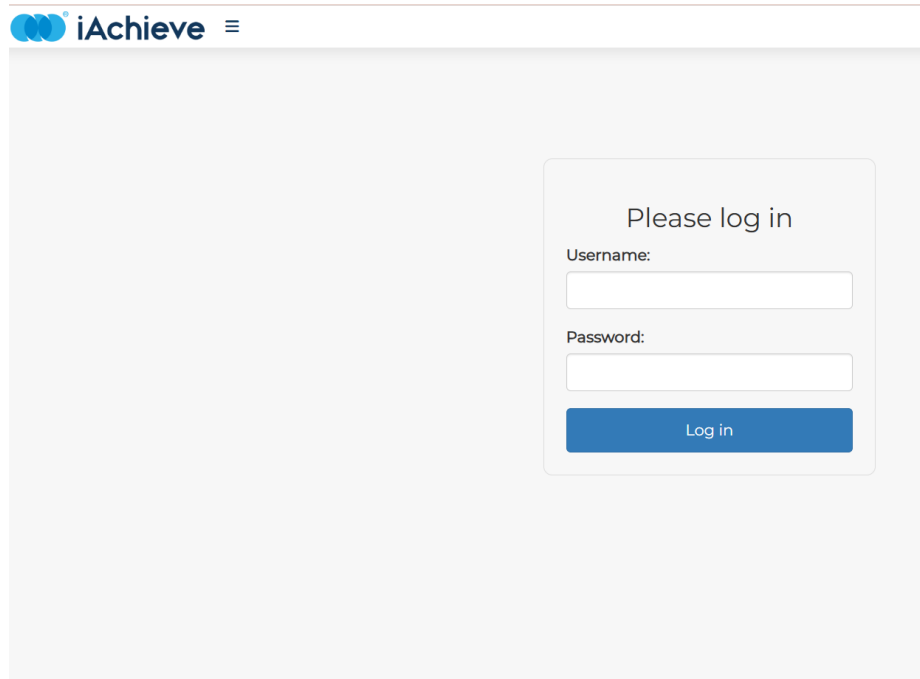


Figure 2 | Launch Screen/Login Window with App Loaded

Figure 3 is the main interface that appears after a successful login. Users begin by uploading images and specifying key input parameters, such as the scale factor (**Pixels per metric**) and the **prediction threshold** to control segmentation sensitivity. Under the *Shape & Size-Based Metrics* section, users can select which particle descriptors (e.g., Feret diameter, length, width, circularity, aspect ratio) should be calculated.

The lower half of the interface provides display settings to toggle plot outputs and percentile metrics such as D10, D50, and D90. Users can also choose to visualize the results using histogram, KDE, and rug plots. Once all inputs and options are configured, pressing the **Start Analysis** button initiates image segmentation and metrics extraction.

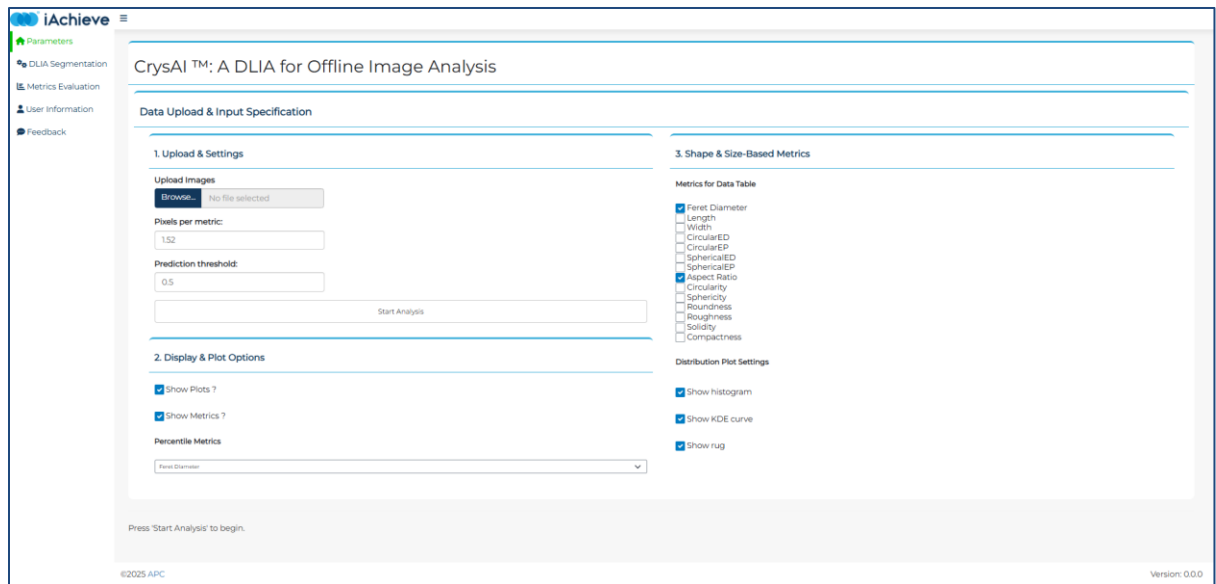


Figure 3 | Homepage of the App – Initial Parameter Specification Page

4. Step-by-Step Instructions

Step 1: Upload & Settings: Upload Image Files

- 1) Click “Upload Images”
- 2) Choose one or more `.jpg` or `.png`, or `.tif` files
- 3) The number of image files added is displayed in the Upload Panel (Figure 4)

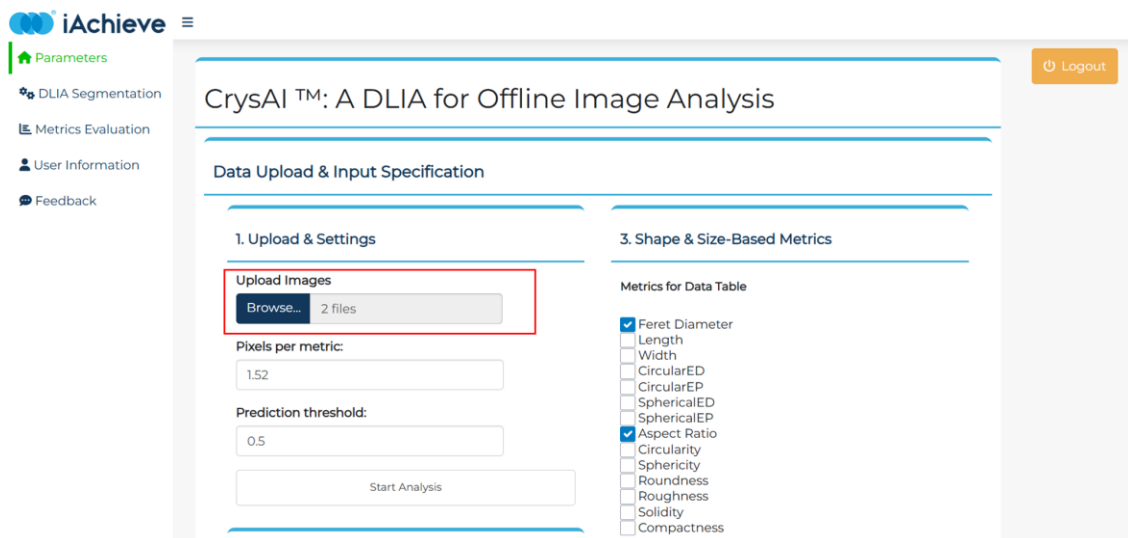


Figure 4 | Screenshot of Upload Panel with number of Image Files,

[Insert Figure 4: Screenshot of Upload Panel with Image Files Loaded]

Step 2: Set Analysis Parameters

1. **Pixels per Metric:** Enter scale (e.g., 1.52 pixels per micron)
2. **Prediction Confidence Threshold:** Adjust using up/down arrow (default: 0.5)
3. **Display & Plot:** Click on Check boxes to Show Plots and/or Metrics Data Table
4. **Percentile Metrics:** Select the desired metrics from the drop down to display D [10], D [50], and D [90] after the analysis (Figure).

2. Display & Plot Options

☒ Show Plots ?

☒ Show Metrics ?

Percentile Metrics

Feret Diameter

- Feret Diameter
- Length
- Width
- CircularED
- CircularEP
- SphericalED
- SphericalEP
- Aspect Ratio
- Circularity
- Sphericity
- Roundness
- Roughness
- Solidity
- Compactness
- Feret Diameter

Figure 5 | Display & Plot Options: Plots, Metrics Table, and Percentile Metrics

5. **Shape & Size-Based Metrics:** Select Metrics to View in Data Table (Check boxes for Length, Width, Aspect Ratio, Circularity etc.); and Distribution Plot Settings: Check boxes to Show Histogram, Kernel Density Estimate (KDE) plots, and rug plots of selected Shape and Size based metrics to view after the analysis is completed (Figure 6).

3. Shape & Size-Based Metrics

Metrics for Data Table

- ☒ Feret Diameter
- ☐ Length
- ☐ Width
- ☐ CircularED
- ☐ CircularEP
- ☐ SphericalED
- ☐ SphericalEP
- ☒ Aspect Ratio
- ☐ Circularity
- ☐ Sphericity
- ☐ Roundness
- ☐ Roughness
- ☐ Solidity
- ☐ Compactness

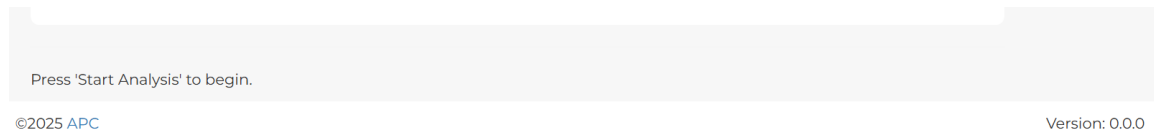
Distribution Plot Settings

- ☒ Show histogram
- ☒ Show KDE curve
- ☒ Show rug

Figure 6 | Panel Showing Input Fields for Metric Selection for the Data Table and Distribution Plots

Step 3: Run Analysis

1 Before starting the analysis, the status bar of the app shows the message “Press Start Analysis to begin”:



2 Click “Start Analysis” button to begin:

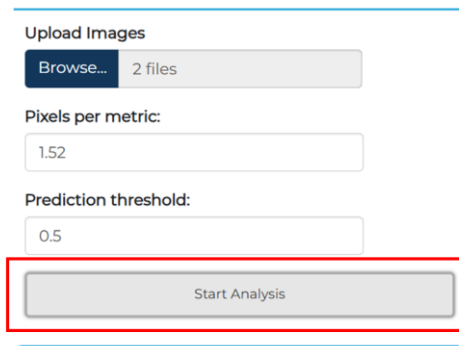
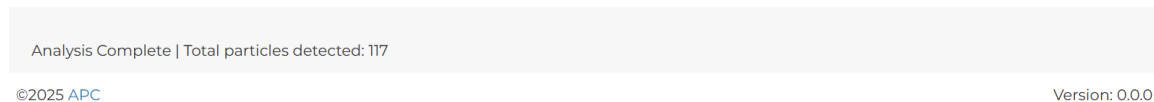


Figure 7 | Panel Showing “Start Analysis” action button

3 Once the analysis is Completed, the status bar displays a summary of the analysis:



Step 4a: View Results: DLIA Segmentation

Once the analysis is completed, navigate to the **DLIA Segmentation** tab in the sidebar (Figure 8).

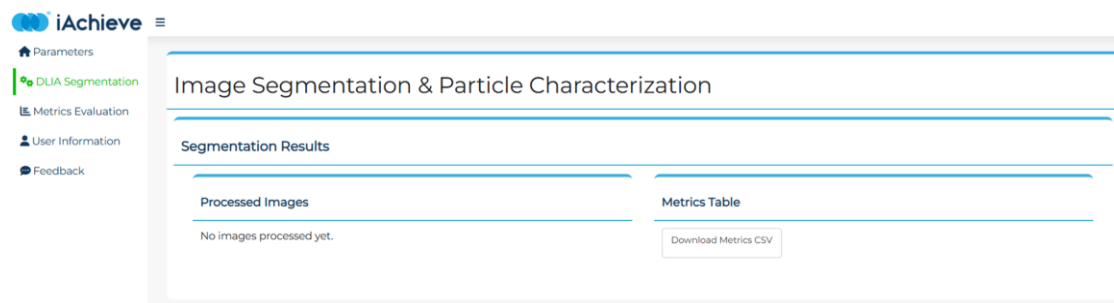


Figure 8 | DLIA Segmentation Tab before Analysis

This section displays the **Segmentation Results**, including overlay images where each particle is highlighted with a mask to visually confirm detection accuracy. Alongside the visual output, a **Metrics Table** is generated, listing shape and size descriptors for each segmented particle — such

as Feret diameter, aspect ratio, circularity, and more. The table can be downloaded as a CSV file for further review, reporting, or integration with downstream analysis workflows.

1 Processed Images: Shows particles with masks (color-coded for different instances of particle counts)

2 Metrics Table: Interactive table of all metrics (The number of shape and size-based elements displayed in Table can be increased or decrease by going back to the Metric selection checkbox group in Parameters Tab (See Figure 6). Figure 9 shows the processed images (segmented with mask overlays) and the Metrics Table.

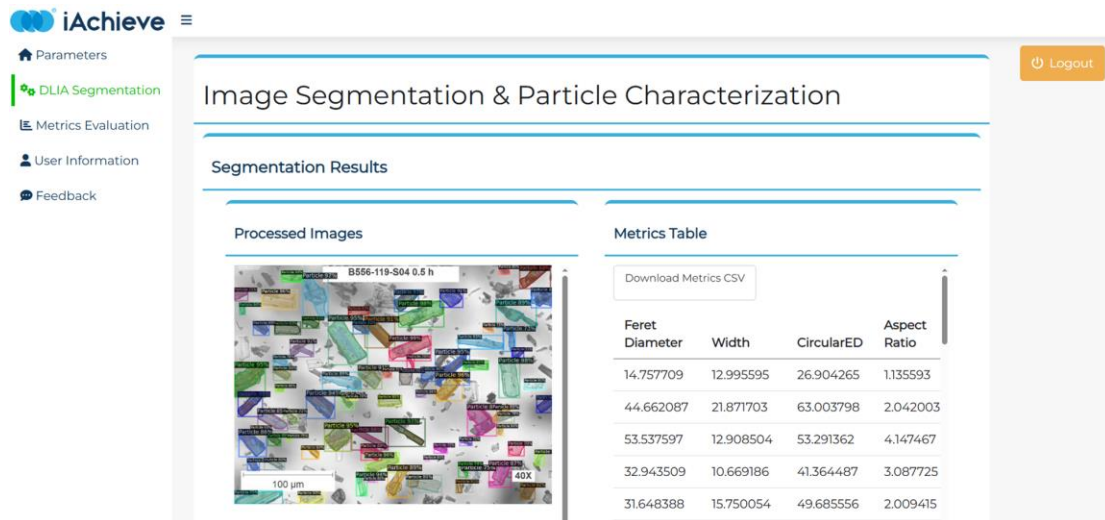


Figure 9 | DLIA Segmentation Results: Processed Images and Metrics Table

Step 4b: View Results: Metrics Evaluation

The **Metrics Evaluation** tab displays summary statistics (i.e. D[10], D[50], and D[90]) and distribution plots for both size-based and shape-based particle descriptors. Figure

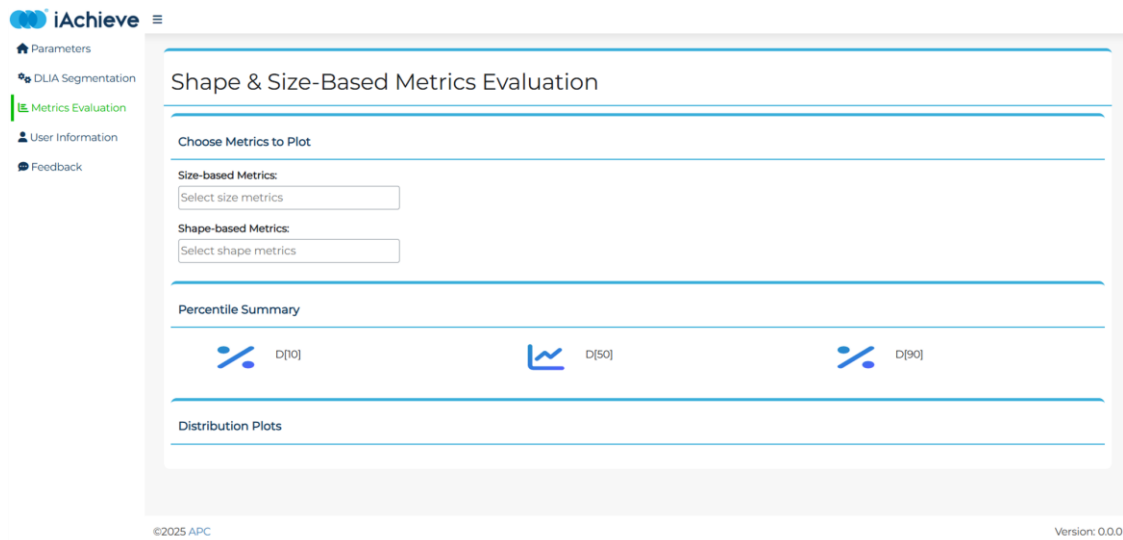


Figure 10 | Metrics Evaluation Tab before analysis

1 Percentile Summary: The app calculates and displays key percentile values—**D10**, **D50**, and **D90**—in the **Percentile Summary** section, giving a quick overview of the metric distribution based on the metrics selected in the **Percentile Metrics** drop down during parameter specification step (see **Figure 5, Step 2**). **Figure 11** shows the summary of the **D[10]**, **D[50]**, and **D[90]** of the Aspect Ratio.



Figure 11 | Metrics Evaluation Tab: Percentile Summary of the Aspect Ratio

2 Distribution Plots: Size and Shape-Based Metrics of interest can be selected from the respective dropdown menus (**Figure 12** and **Figure 13** respectively). The **Distribution Plots** section renders the data visually using histograms, Kernel Density Estimate (KDE) curves, and rug plots, depending on the display options set in the Shape-based and Size-based selection tabs shown in **Figure 12**.

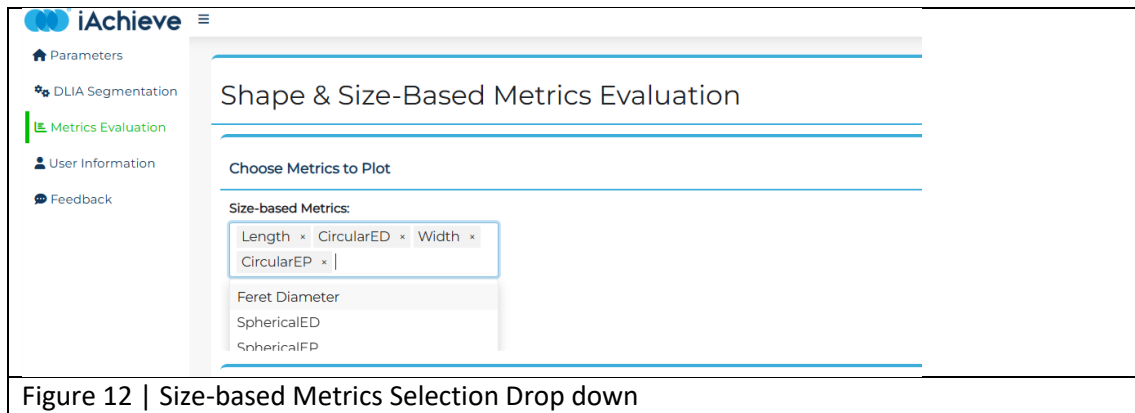


Figure 12 | Size-based Metrics Selection Drop down

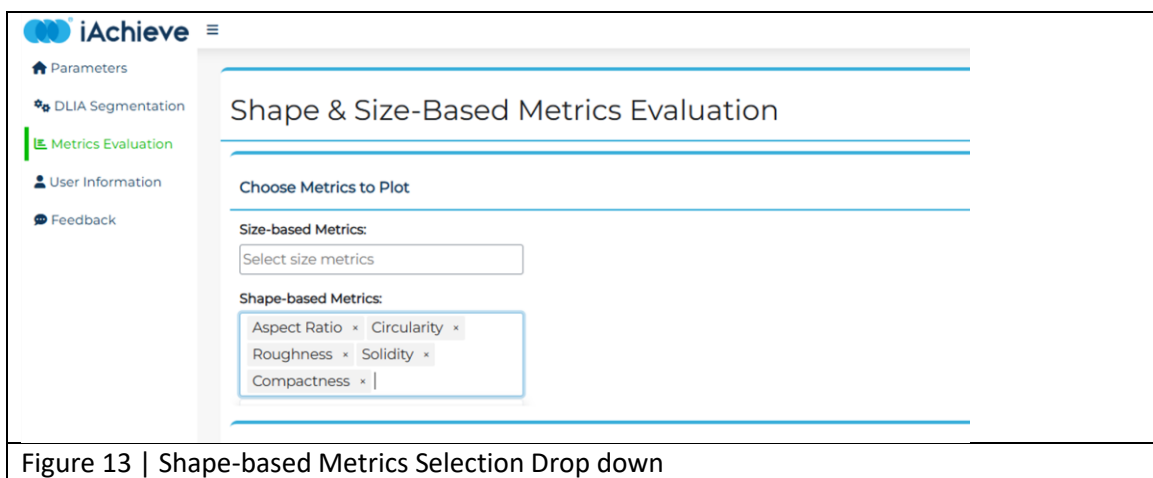


Figure 13 | Shape-based Metrics Selection Drop down

Figure 14 shows the distribution for each selected size and shape-based metric, facilitating a deeper understanding of particle morphology variations.

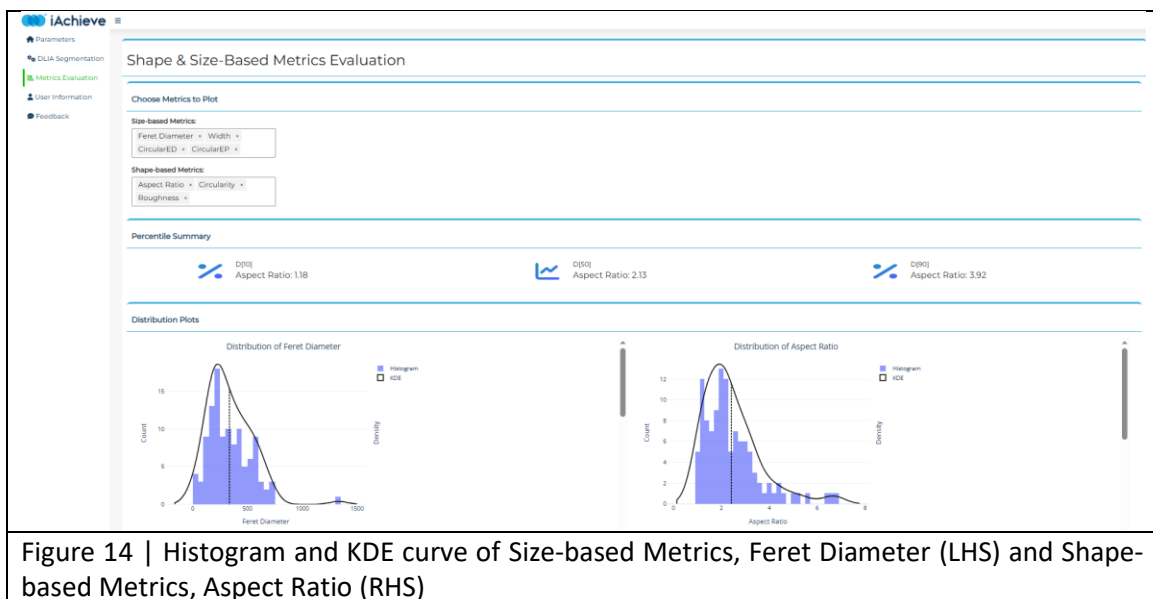


Figure 14 | Histogram and KDE curve of Size-based Metrics, Feret Diameter (LHS) and Shape-based Metrics, Aspect Ratio (RHS)

Step 5: Export Results

1 Use “Download CSV” button to save Metrics Table as `.csv` (Figure 15).

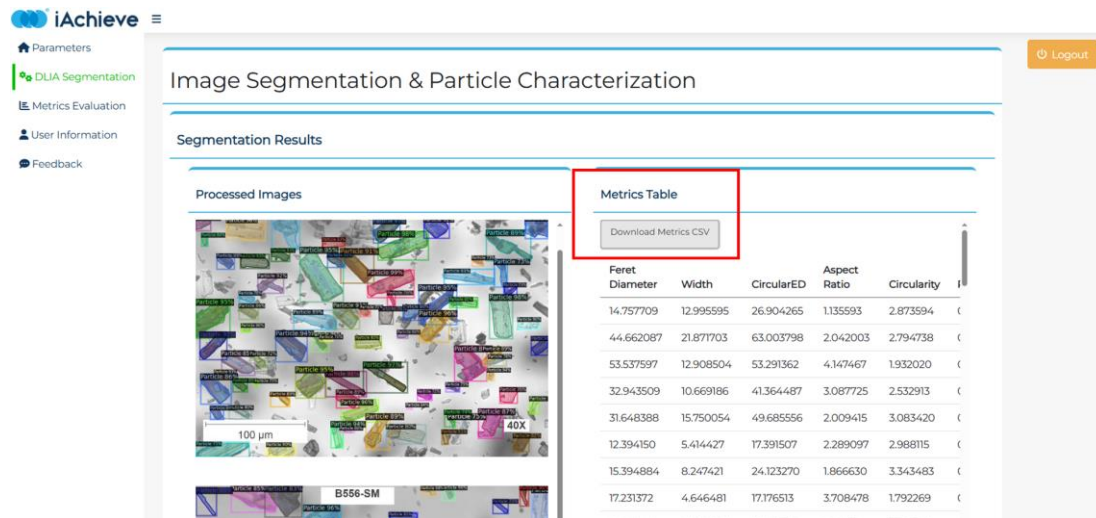


Figure 15 | Metrics Table Download Button

2 Use download tool on the Distribution plots to save distributions and histograms

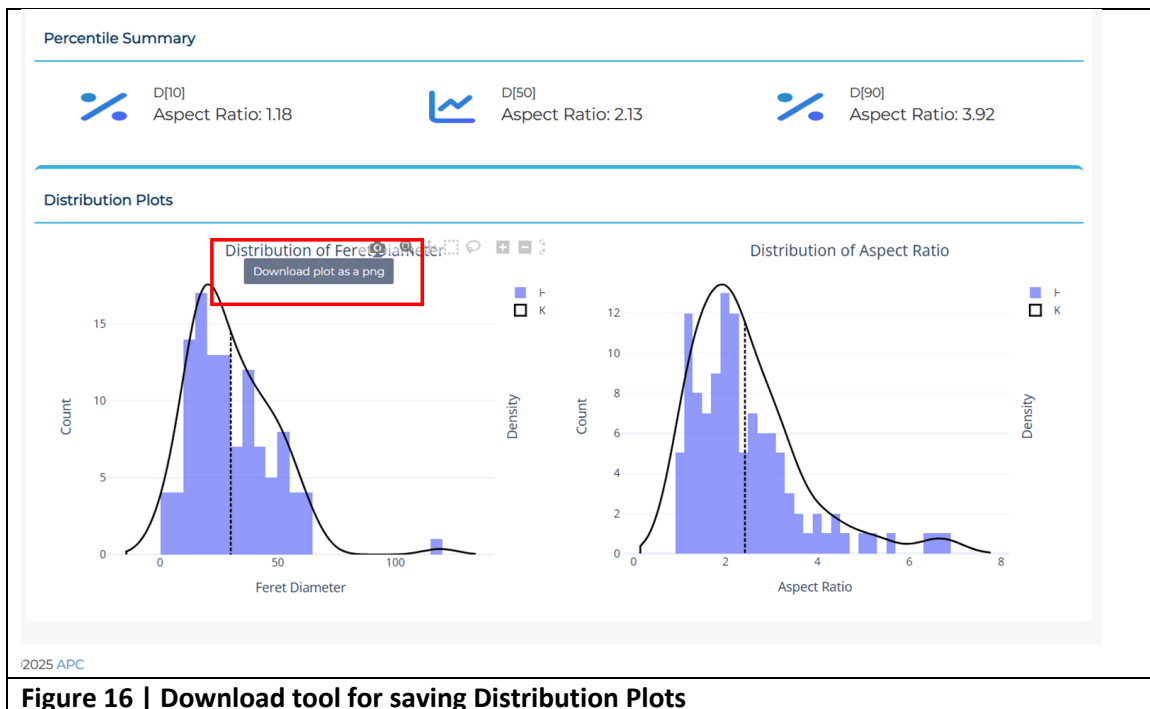


Figure 16 | Download tool for saving Distribution Plots

5. Sample Output Shape & Size-Based Metrics Explained

Metric	Description
Length	Maximum Feret diameter
Width	Minimum Feret diameter
Aspect Ratio	Ratio of length to width
Circularity	$4\pi \times (\text{Area} \div \text{Perimeter}^2)$
Area	Number of pixels enclosed by the particle
D10/D50/D90	Size/Shape percentiles of particle distribution

[Insert Figure 17: Annotated Diagram of a Particle Showing Length, Width, Perimeter]

6. Tips and Best Practices

- Use high-contrast, in-focus images
- Apply consistent scale bars and lighting
- Choose a confidence threshold appropriate for noise levels
- Review outputs and adjust parameters if needed

[Insert Figure 18: Example Comparison of Good vs Poor Input Image]

7. Troubleshooting Guide

Common issues and their solutions:

Issue	Resolution
No particles detected	Lower threshold slider
Particles too small or merged	Increase image resolution
Wrong scale	Double-check pixels per metric value
Outputs not appearing	Ensure all inputs are filled before clicking Start

[Insert Figure 19: Example of App Showing No Output and Input Error Message]

8. Support

For help or questions, Fill the **Feedback Form** on the App with your **email address** and **queries**.
Sample input files and FAQs are available in the shared folder.