

Software Requirements Specification for ImgBeamer: Scanning Electron Microscope Image Formation

Joachim de Fourestier

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Revision History

| Date | Version | Notes |
|------------|---------|---|
| 2023/02/03 | 1.0 | First version |
| 2023/02/11 | 1.1 | Changes after review by domain expert |
| 2023/02/15 | 1.2 | Changes after review by SRS secondary reviewer |
| | 1.3 | Includes some changes after review by Dr. Smith |
| 2023/02/17 | 1.3.1 | Added some missing definitions |
| | 1.3.2 | Some changes needed for use with the VnV plan |
| 2023/02/20 | 1.3.3 | Tweaks some definitions, some math notation updates |
| 2023/02/22 | 1.3.4 | Define RMSPE-based image metric. |
| | 1.3.5 | Add 8-bit depth grayscale as a system constraint. |
| 2023/03/04 | 1.3.6 | Use NRMSE as the main term instead of RMSPE. |

1 Reference Material

This section records information for easy reference.

1.1 Table of Units

Throughout this document SI (Système International d’Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the name.

| symbol | unit | name |
|---------------|--------|---------------------------|
| px | pixel | picture element |
| nm | length | nanometre (10^{-9} m) |
| μm | length | micrometre (10^{-6} m) |

1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The choice of symbols was made to be consistent with EM (Electron Microscopy) literature and with existing documentation for EM systems. The symbols are listed in alphabetical order.

| symbol | unit | description |
|------------------|------------------|---|
| d_p | nm | probe diameter (size) |
| d_i | nm | probe step size in image space |
| d_o | nm | probe step size in object space |
| η | dimensionless | BSE yield |
| δ | dimensionless | SE yield |
| α_q | dimensionless | Image quality metric (see 2) |
| $I_{n \times m}$ | 8-bit gray level | Image intensity matrix that has n rows and m columns. |
| $M_{n \times m}$ | Boolean | Mask / stencil matrix that has n rows and m columns. |
| $R_{n \times m}$ | 8-bit gray level | Resulting image intensity matrix that has n rows and m columns. |
| $G_{n \times m}$ | dimensionless | A matrix representation of the raster or imaging grid that has n rows and m columns. |
| $i_{x,y}$ | dimensionless | An entry (at x, y) in the raster grid represented by an intensity or signal value. |
| $m_{x,y}$ | Boolean | An entry (at x, y) in a mask matrix. |
| $r_{x,y}$ | dimensionless | An entry (at x, y) in the resulting image represented by an intensity or signal value. |

1.3 Abbreviations and Acronyms

| symbol | description |
|-----------|-------------------------------------|
| 2D | two-dimensional |
| 3D | three-dimensional |
| A | Assumption |
| BSE | Backscattered Electron |
| CCD | Charge Coupled Device |
| DD | Data Definition |
| EM | Electron Microscopy |
| FOV | Field of View |
| GD | General Definition |
| GS | Goal Statement |
| IM | Instance Model |
| LC | Likely Change |
| LM | Light Microscopy |
| PS | Physical System Description |
| R | Requirement |
| ROI | Region of Interest |
| RMSE | Root Mean Square Error |
| NRMSE | Normalized Root Mean Square Error |
| RMSPE | Root Mean Square Percentage Error |
| SE | Secondary Electron |
| SEM | Scanning Electron Microscope |
| SRS | Software Requirements Specification |
| TM | Theoretical Model |
| ImgBeamer | SEM image formation demo tool |

2 Introduction

Images formed by SEM (Scanning Electron Microscope) are created using a specific process where the image quality can be greatly influenced by the imaging parameters (e.g., spot profile, pixel size). Since the quality of an image is very often evaluated subjectively by an experienced microscope user, the motivation of this software project “ImgBeamer” is to provide a way to visualize qualitatively the said influence without the need of a physical instrument. Incorrectly adjusting the imaging parameters could lead to a loss of information or misinterpretation. The issue is further explained in the Problem Statement document. Some figures expanding on the subject can be found in section 4.1.2. An underlying goal is also to prove or disprove if there is a “rule of thumb” for the optimal spot-to-pixel size ratio.

2.1 Purpose of Document

This document serves as the software requirements specification. The details of the requirements, limitations, definitions, models to be used are laid out explicitly within this document.

2.2 Scope of Requirements

The scope of the requirements is restricted to only the image formation process used in SEMs, more specifically the image processing from signal to an image or visual representations. It does not cover electron-sample interactions or CCD (charge-coupled device) detector voltage to signal value conversion. See the assumptions section (Section 4.2.1) for further details.

2.3 Characteristics of Intended Reader

The intended reader of this document should have a basic understanding of electron-optics concepts used by an SEM. This can be equated to standard level two university physics (optics, electricity, magnetism, thermodynamics and modern physics) along with a standard undergraduate course related to materials characterization (concepts such as backscattered electrons, mean free path, and electron density). The reader should have a basic understanding of two-dimensional image processing techniques and level one university linear algebra (matrices).

2.4 Organization of Document

This document contains an introduction to the software and its goals. It is meant to be a reference document to the readers and is based on an SRS template from [Smith and Lai \(2005\)](#); [Smith et al. \(2007\)](#). The document includes a description of the scope, a detailed list of the terminology, definitions, and models used, as well as a more specific and detailed description of the problem and its solutions. This document also defines the requirements, as well as the likely changes and traceability details.

3 General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

3.1 System Context

The general input and output pattern of the ImgBeamer software is shown in the system context diagram (figure 1). This section also includes the responsibilities of the user and the software.

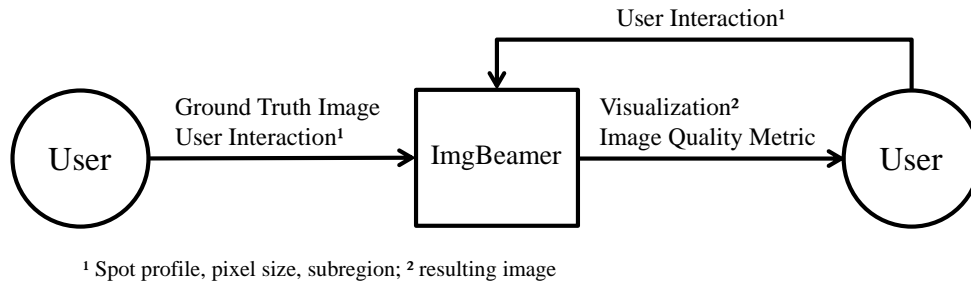


Figure 1: System Context

- User Responsibilities:
 - Provide an image of sufficient size (see 4.2.6), such that there is enough detail.
 - Provide a ground truth image that should be free of distortions (e.g., from FOV edges, depth of field, “charging”, insufficient focus, astigmatism, etc.).
 - Be able to interact with the software’s graphical user interface using a computer mouse, keyboard and monitor.
 - Provide realistic spot profiles (size and shape).
 - Run the software on a platform or system with sufficient resources to process computer graphics.
- ImgBeamer Responsibilities:
 - Provide the ability load or change the input ground truth image.
 - Detect and warn about invalid or corrupt image files.
 - Set reasonable limits (minimum and maximum dimensions) on the spot profile.
 - Be responsive, taking user input at anytime and prevent locking or freezing of the graphical user interface as much as possible.
 - Have reasonable starting default inputs and values.
 - Display the image quality metric.
 - Provide the ability to export the resulting images.

3.2 User Characteristics

The ImgBeamer software end user is anyone that has used an SEM or is learning about them. This ranges from a university undergraduate science student whose curriculum includes EM (Electron Microscopy), to experienced SEM operators or even to experts in the field of EM. The software end users also include those described in Section 2.3 (intended readers of this document). That said, neither image processing nor linear algebra knowledge is required to use the software.

3.3 System Constraints

The real world design constraints are to be listed here. Currently, the only constraint is that images will be restricted to 8-bit grayscale (as listed in Table 3).

4 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models.

4.1 Problem Description

ImgBeamer is intended to help visualize and understand the influence of the spot profile and pixel size. It should be able to help determine the optimal spot-to-pixel-size ratio (see fig. 4 and 5).

4.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

| Terminology | Definition |
|------------------------|---|
| Backscattered Electron | An electron that is elastically scattered backwards to the initial direction of travel as a result of electron-sample interactions between the beam and the sample. |
| Beam | The continuous focused stream of electrons accelerated at high speeds down the column of an electron microscope. |

| | |
|------------------------------|---|
| Bit Depth | It is the range of the value (intensity or color) of a pixel. Specifically, it is the maximum number of bits used to represent said value. |
| Brightness | The intensity value (or perceived luminance for colours) of a signal, point (or pixel), or area within an image. |
| Contrast | The difference or distinguishable quality of an intensity (or colour) or brightness value of a point (or pixel) from another point in an image. |
| Electron-Sample Interactions | The interactions as a result of electrons from the beam hitting the sample surface leading to an electron collision cascade. This in produces various emissions such as x-rays, BSEs, and SEs. |
| Electron Microscopy | The practice of microscopes that specifically use electrons as the source of illumination to produce an image or signal. |
| Exact-sampling | The sampling size or rate that matches the specificity of the targeted resolution. In the context of this document, this is when the size of the probe that matches the size of the pixel. |
| Field of View | The observable or visible extent given by the microscope and varies with magnification. |
| Ground Truth | The data or information that is considered as the source or reference standard of truth. |
| Image | A representation of visual information that can be represented by 2D matrix where each cell represents a pixel with a specific value (representative of intensity or colour). – |
| Image Quality | The perceived clarity, amount of information or detail representative of reality that is contained within an image. |
| Image Resolution | The size dimensions (width and height) of an image. Typically, it is defined in pixels. |
| Interaction Volume | The volume within the sample in which there are electron-sample interactions caused by the beam coming into contact with the surface of the sample. |
| Light Microscopy | The practice of microscopes that specifically use light as the source of illumination to produce an image or signal. |
| Mean Free Path | The average distance within a system that a particle can travel before it collides with other particles. |
| Nyquist Limit | More formally known as the “Nyquist-Shannon” sampling limit is the minimum sampling rate at which all the essential information is captured when discretizing a continuous signal, resulting in little to no distortions. |

| | |
|-----------------------|---|
| Over-sampling | This is a sampling rate or size that is too large where the specificity or origin of the information is lost. This generally results in increased confidence, but at a loss of precision. |
| Pixel Size | The size or dimensions of one cell within a raster grid. |
| Probe | Generally interchangeable with “beam”. Contextually within this document, it is the final part of the beam that comes into contact with the surface of the sample (being analyzed within the microscope) forming a “spot” with a targeted size and shape. |
| Raster Grid | An imaging grid or scanning pattern with a defined and repeated cell size. |
| Region of Interest | A defined 2D area in both position, size, and shape on a sample. |
| Resolution | As defined by the Rayleigh criterion, it is the minimum distance by which two points or features can be distinguished. |
| Secondary Electron | An electron that emitted from the sample as a result of inelastic electron-sample interactions between the beam and the sample. These can be weakly bounded valence electrons or conduction band electrons. |
| Signal-to-Noise Ratio | The amount of information (signal) considered useful or representative of reality versus the amount of noise. |
| Spot Content | The information or content from an area covered and sampled by the probe to produce a signal value. |
| Spot Layout | The regular arrangement, sizing, and positioning of the spots and the raster grid used for imaging the sample surface. (ex. see fig. 3) |
| Spot Profile | The combined properties of the <i>Spot Size</i> , the <i>Spot Shape</i> , and the angle of rotation of the spot. |
| Spot Shape | The overall shape of the spot or probe, whether is it a perfect circle or elongated ellipse, or even a halo or ring. |
| Spot Size | The overall diameter or average feret/caliper diameter of the probe. |
| Step Size | The length or distance of a “pixel” by which the probe is moved or deflected when raster scanning the surface of a sample. |
| Subregion | A rectangular region or area usually contained within the current FOV. This can also be synonymous to rectangular ROI. |
| Under-sampling | This is a sampling rate or size that is too small where the specificity or origin of the information is more restricted. This generally results in increased precision, but at a loss of confidence, or even accuracy. |

4.1.2 Physical System Description

The basic principle of the SEM image formation process is to scan an electron beam over the surface of the sample (fig. 2) at discrete locations: cells of a raster or scan grid. A signal (e.g., BSEs, SEs) is produced as the beam dwells over each cell (representing a pixel in the resulting image). This signal is then collected by detectors to calculate a value (or intensity) to fill the corresponding pixel in the resulting image. The area sampled (spot content) depends on the spot's (produced by the beam) size and shape (see fig. 3).

The physical system of ImgBeamer, as shown in Figure 2 and 3, includes the following elements:

PS1: The sample that is being imaged or studied.

PS2: An SEM that includes a BSE and/or SE detector. The electron beam interacts with the sample surface in high-vacuum producing various signals.

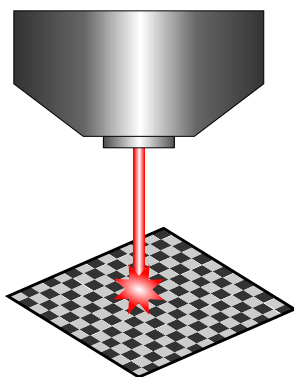


Figure 2: Schematic drawing of an electron beam hitting the sample surface within an SEM chamber. (Image from: <https://github.com/joedf/ImgBeamer>)

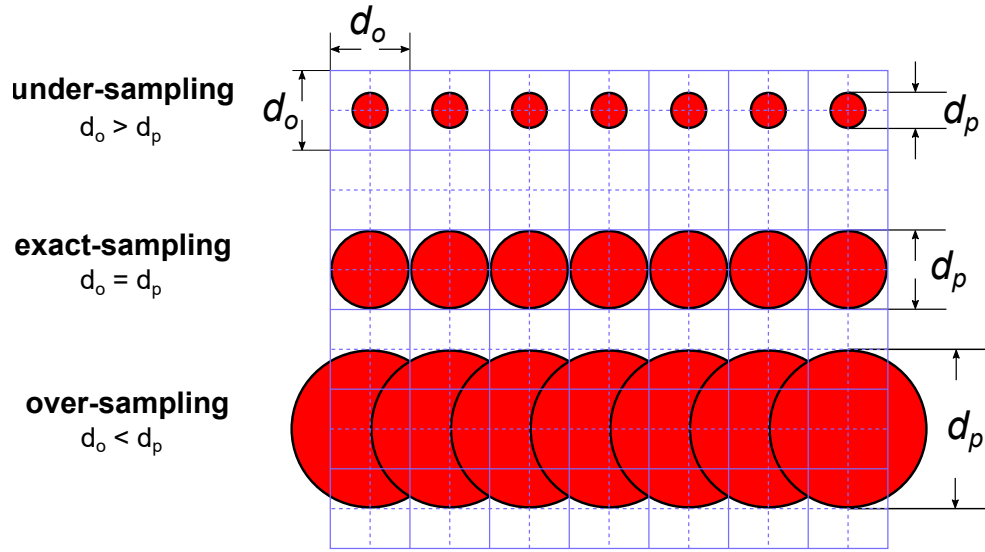


Figure 3: Schematic of the three sampling scenarios (under-sampling, exact-sampling, and over-sampling) and a visual representation of the pixel grid, d_p , and d_o . The dashed lines are to help visualize the center of each pixel cell. Adapted from Lifshin et al. (2014)

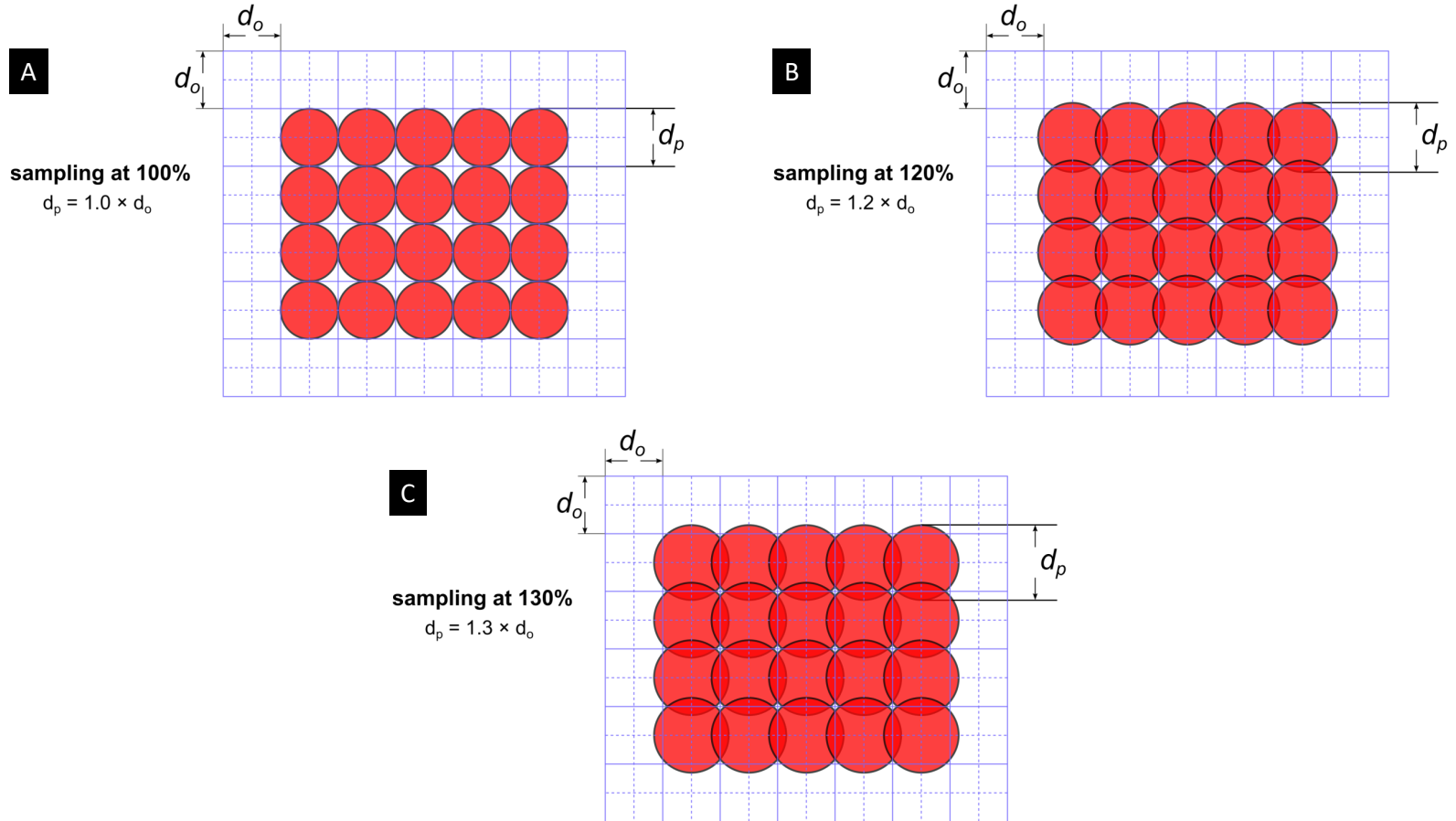


Figure 4: Different scenarios of the spot sizes (represented by the red circles) are presented to show the area coverage and overlap that would occur in a raster scan. [A] represents exact-sampling (as explained in figure 3), where there are considerable gaps between the spot locations. In [B], the gaps are small meaning little loss in area coverage, but there is some overlap. In [C], as we approach to a spot diameter that is equal to the square diagonal ($\sqrt{2} \approx 1.4142$), the gaps are significantly reduced as the overlap grows to a geometric maximum.

Depending on how large the spot size is, the surface area coverage (or spot content) will vary. As shown in figure 4, a circular spot cannot cover the entire area without overlap. However, when the spot size is small, there is no overlap, but there are significant gaps where potentially means a loss of information. There is a balance between the overlaps and the gaps. In figure 5, we can see how this balance can affect the reconstructed image's sharpness versus its amount of detail or visual information.

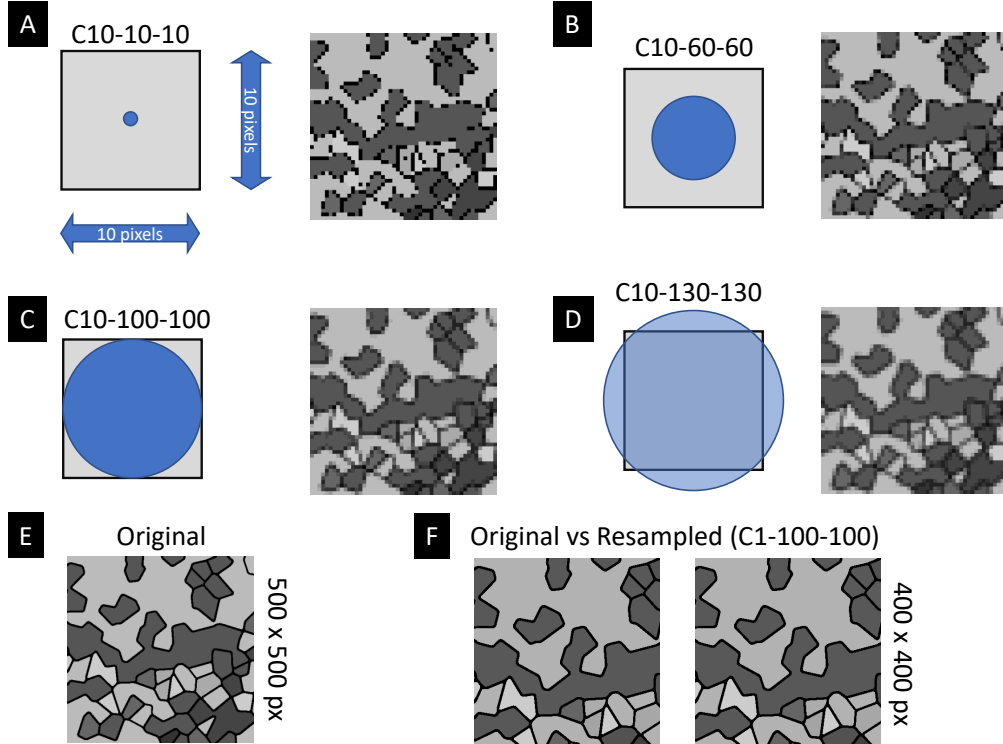


Figure 5: Different sampling scenarios are presented here (A-D). The blue circles represent the imaging or beam spot. The notation C10 represents a square cell size of 10 by 10 pixels. The following numbers are percentages of the spot diameter size with respect to the cell width. For example in [D], we have a spot where its diameter is 130% of the cell's width. [E] represents the original image that was resampled. It is a virtual BSE image representing a crystalline sample. [F] shows a “high-fidelity” reconstructed image meaning the pixel size is one-to-one with exact-sampling (100%). There is no perceivable difference.

In more extreme cases as shown in figure 6 (exaggerated for clarity), if there is over-sampling in one direction and under-sampling in another, it can create the effect of astigmatism. Whereas in the scenario where we grossly over-sample in all directions, we obtain the effect of an unfocused image.

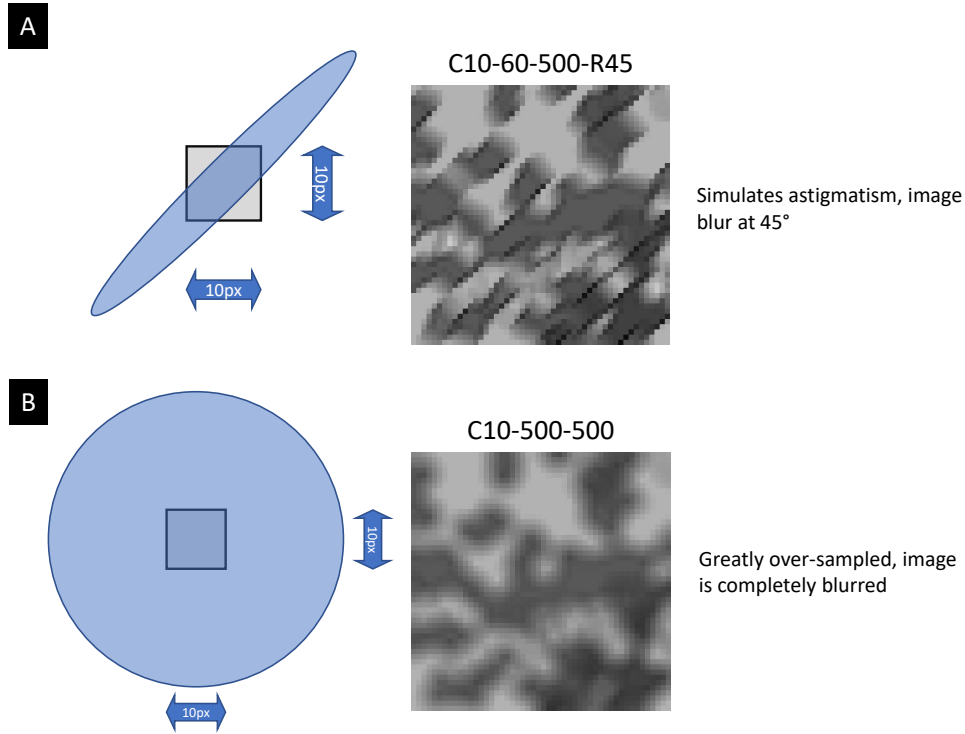


Figure 6: Following the same notation as explained in figure 5, here are two extra examples (A and B). [A] represents the scenario of astigmatism that is dominant at a 45-degree angle. [B] represents the scenario of defocus (or insufficient focus).

4.1.3 Goal Statements

Given an image (ground truth) and imaging parameters (e.g., spot size, spot shape, pixel size), the goal statements are:

GS1: Reprocess the image following the SEM image formation process.

GS2: Provide a quantitative metric of relative image quality of the resulting image.

GS3: Visualize the effects of changing the imaging parameters.

GS4: Export the reprocessed images.

4.2 Solution Characteristics Specification

This section provides the assumptions, instance models, theoretical models, general definitions, and data constraints. The information specified in this section is intended to reduce ambiguities and reduce the problem into clear logical or mathematical terms.

The instance models that govern ImgBeamer are presented in Subsection 4.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

4.2.1 Assumptions

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [TM], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: The sample surface is solid.

A2: The sample material is made of atoms with atomic numbers greater than 3 (lithium and lighter elements are not detectable in SEM).

A3: The electron beam is ideal (meaning stable and collimated meaning all the electrons are traveling parallel to each other down towards the sample surface within high vacuum for optimal mean free path).

A4: The input image of the sample is considered to have infinite resolution representative of reality: ground truth.

A5: The signal yields (such as BSEs and SEs, see DD1) are high enough to produce an image meaning optimal SNR (enough signal, contrast [TM2] and noise is low).

A6: The image produced by the SEM (see DD2) as the electron raster scan the sample surface is an approximate representation of reality.

A7: The beam's deflection space (TM4) will not be a limiting factor in how wide the coverage area of the sample surface.

4.2.2 Theoretical Models

This section focuses on the general equations and laws that ImgBeamer is based on.

| | |
|-------------|---|
| Number | TM1 |
| Label | Mean Free Path |
| Equation | $\lambda = \frac{RT}{\sqrt{2}\pi d^2 N_A P}$ |
| Description | <p>λ is the mean free path (m)</p> <p>R is the universal gas constant = 8.3145 J/mol K</p> <p>T is the temperature (K)</p> <p>d is the molecular diameter (m)</p> <p>P is the pressure (Pa)</p> <p>N_A is Avogadro's number = $6.0221 \times 10^{23} \text{ mol}^{-1}$</p> |
| Notes | See A3. |
| Sources | http://hyperphysics.phy-astr.gsu.edu/hbase/Kinetic/menfre.html |
| Ref. By | — |

| | |
|-------------|---|
| Number | TM2 |
| Label | Contrast |
| Equation | $C_{tr} = (S_2 - S_1)/S_2$ |
| Description | <p>C_{tr} This is proportion or level of contrast or difference in signal. It is dimensionless.</p> <p>S is the emitted signal strength or intensity (see DD1).</p> <p>S_1 is one signal at one location (e.g., pixel).</p> <p>S_2 is another signal at a different location to be compared with S_1 and should the larger value of the two signals.</p> |
| Notes | $S_2 > S_1$ |
| Sources | Goldstein et al. (2018b) , Lifshin et al. (2014) |
| Ref. By | A5 |

| | |
|-------------|--|
| Number | TM3 |
| Label | Magnification |
| Equation | $M = \frac{d_i}{d_o}$ |
| Description | <p>M is the magnification ratio (unitless)</p> <p>d_i is the probe step size in image space</p> <p>d_o is the probe step size in object space</p> |
| Notes | The input (ground truth) should be large enough and sufficient detail, see A4. |
| Sources | Lifshin et al. (2014) |
| Ref. By | – |

| | |
|-------------|---|
| Number | TM4 |
| Label | Deflection Space (or area / field) |
| Description | <p>The deflection space is the area bounds in which the beam can be redirected or oriented using deflection coils. It can be expressed in real world units, but this can vary between SEMs.</p> <p>From an imaging perspective, it can be generalized as a normalized unit square coordinate system where the top left is (-0.5, -0.5), the center is (0.0, 0.0), and the bottom right is (0.5, 0.5).</p> |
| Source | Goldstein et al. (2018a) |
| Ref. By | A7, GD1 |

4.2.3 General Definitions

This section collects the laws and equations that will be used in building the instance models.

| | |
|-------------|---|
| Number | GD1 |
| Label | Raster or Scan Grid |
| Units | px (pixels) |
| Equation | $G_{n \times m}(x, y) = i_{x,y} \{0 \leq x \leq m, 0 \leq y \leq n\}$ |
| Description | <p>G is the grid applied to the sample surface (can be represented as a matrix) spanning within deflection space (TM4) of the SEM.</p> <p>Each cell is a discrete (x, y) location over which the beam scans over to produce a signal. These signals are then collected by detectors to generate an image.</p> <p>Each cell $(i_{x,y})$ represents a picture element or “pixel” with an intensity or signal value.</p> <p>By convention, pixels are square, but this is not a necessity. That said, non-square pixels may lead to unfaithful or distorted representations, see A6 and Goldstein et al. (2018a).</p> <p>The size of a pixel can be expressed in nm, μm, or even a percentage of the FOV.</p> |
| Source | Goldstein et al. (2018a) |
| Ref. By | — |

4.2.4 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.

| Number | DD1 |
|-------------|---|
| Label | Signal yield / intensity |
| Symbol | η (for BSE), δ (for SE), Y (for general) |
| Units | dimensionless |
| Equation | $Y_{signal} = N_{signal}/N_B$ |
| Description | <p>Y_{signal} is the intensity relative to the incident beam.</p> <p>N_{signal} is the number of scattered or emitted electrons.</p> <p>N_B is the number of (primary) incident electrons from the beam.</p> |
| Notes | <p>The <i>signal</i> can BSE or SE.</p> <p>There assumptions related to the beam, the signal produced, and sample nature, see A2, A3, and A5.</p> |
| Sources | Goldstein et al. (2018b) |
| Ref. By | DD2, TM2, A5 |

| Number | DD2 |
|-------------|---|
| Label | Signal Image |
| Symbol | $I_{n \times m}$ |
| Units | intensity / ratio - unitless |
| Description | <p>Each cell represents a pixel with a signal intensity (see DD1) or brightness value where the range depends on the bit depth.</p> <p>A bit depth of 8 is 0 to 255 (0xFF), and 16 is 0 to 65535 (0xFFFF).</p> <p>We assume (see A5) there's enough signal that can be detected, as a 0 represents no or “undetected” signal.</p> |
| Sources | Goldstein et al. (2018b) |
| Ref. By | IM1, A6 |

4.2.5 Instance Models

This section transforms the problem defined in Section 4.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.

The goal of reprocessing an image GS1 will be solved by IM1. The goal of providing an image quality metric will be solved by IM2.

| | |
|-------------|---|
| Number | IM1 |
| Label | Bit BLT (as known as Bit Block Transfer) |
| Input | an image $I_{n \times m}$ and a mask $M_{n \times m}$ |
| Output | reprocessed image $R_{n \times m}$ |
| Description | <p>Given an image (see DD2) and mask (or stencil), a boolean operation is performed iteratively on each cell of the image matrix, based on the corresponding cell value found in the mask matrix at row x and column y.</p> $r_{x,y} = \begin{cases} i_{x,y} & \text{if } m_{x,y} = \text{True} \\ 0 & \text{otherwise} \end{cases}$ <p>If the mask cell value ($m_{x,y}$) is True, the corresponding image cell value is transferred/kept in the resulting/destination matrix, meaning $r_{x,y} = i_{x,y}$.</p> <p>Otherwise, if the corresponding mask matrix cell ($m_{x,y}$) is False, then no value is transferred, and zero will be inserted at x, y in the destination image matrix, meaning $r_{x,y} = 0$.</p> |
| Sources | Pike et al. (1984), https://en.wikipedia.org/wiki/Bit_blit |
| Ref. By | R6 |

| | |
|-------------|---|
| Number | IM2 |
| Label | Image quality metric (Inverted NRMSE) |
| Input | an image $I_{n \times m}$ serving as ground truth and the image $R_{n \times m}$ to compare |
| Output | a positive value ranging from 0 to 1.00. |
| Description | <p>Given the original image (ground truth, see A4) and a reprocessed image, a metric must be calculated to express image similarity where 1.00 means a perfect match and 0.00 means absolutely no correlation or similarity found.</p> <p>The metric (α_q) uses normalized RMSE, called NRMSE (eq. 1) or sometimes RMSPE. In this case, the RMSE is normalized using the maximum value possible ($\text{pixel}_{max} = 255$ for 8 bit depth for grayscale images).</p> $\text{NRMSE} = \frac{1}{\text{pixel}_{max}} \cdot \sqrt{\frac{1}{n} \cdot \sum_{i=1}^n (I_i - R_i)^2} \quad (1)$ <p>Where n is the total number of pixels of one image, I_i is a pixel from the ground truth image, and R_i is the corresponding pixel in the result image.</p> <p>Note that $\text{pixel}_{max} = 255$ should be subtracted by $\text{pixel}_{min} = 0$, but is omitted for simplicity.</p> $\alpha_q = 1 - \text{NRMSE} \quad (2)$ <p>The values of the metric (eq. 2) do not need to be absolutely quantitative. They only need to be relatively comparable when only changing d_p or the spot shape.</p> <p>If the images do no match in size, the smaller image shall be scaled to match.</p> |
| Sources | Jagalingam and Hegde (2015), https://cirpwiki.info/wiki/Statistics#Normalization |
| Ref. By | R7, NFR2 |

4.2.6 Input Data Constraints

Table 2 shows the data constraints on the input output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the

variable. The column for software constraints restricts the range of inputs to reasonable values. The software constraints will be helpful in the design stage for picking suitable algorithms. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 2 are listed in Table 3.

Table 2: Input Variables

| Var | Physical Constraints | Software Constraints | Typical Value | Uncertainty |
|-----------|--------------------------|--|---------------|-------------|
| d_p | $d_p > 0.4 \text{ nm}^1$ | $d_{min} \leq d_p \leq d_{max}$ | 10 nm | 10% |
| d_i | $d_i > 0.4 \text{ nm}^1$ | $d_{min} \leq d_i \leq d_{max}$ | 150 nm | 10% |
| n | — | $n_{min} \leq n \leq n_{max}$ | 1024 | 10% |
| m | — | $m_{min} \leq m \leq m_{max}$ | 1024 | 10% |
| $I_{i,j}$ | — | $\forall i, j : 0 \leq I_{i,j} \leq I_{max}$ | 128 | 10% |

¹The reason for this number is that most SEMs cannot achieve finer resolution than this.

Table 3: Specification Parameter Values

| Var | Value |
|-----------|-------------------|
| d_{min} | 0.4 nm |
| d_{max} | 1000 nm |
| n_{min} | 256 px |
| m_{min} | 256 px |
| n_{max} | 4096 px |
| m_{max} | 4096 px |
| I_{max} | 255 (8 bit depth) |

4.2.7 Properties of a Correct Solution

Not applicable, as this is visualization software where the correct or appropriate solution is determined by the user's satisfaction and desired results.

5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

5.1 Functional Requirements

R1: Accept an input image in the following formats:

- PNG (Portable Net Graphics)
- JPG (Joint Photographic Experts Group)
- BMP (Bitmap)
- preloaded example images

R2: Accept user input of the spot profile (size and shape) and ensure that all its defining values are positive real numbers.

R3: Accept user input of pixel size and ensure it is valid (a positive real number).

R4: Accept user input to specify a subregion or ROI for processing.

R5: Display a representative spot layout used for processing the image.

R6: Display and allow the user to export the resulting image (processed using IM1).

R7: Calculate and display an image quality metric (according to IM2) to the user.

5.2 Nonfunctional Requirements

The key nonfunctional requirements of this software are accuracy, usability, maintainability, and portability. These are listed below in detail:

NFR1: **Accuracy** The images produced should be not manipulated to produce results that subjectively represent the opinions of the author(s) or developer(s). Thus, the software should transparently follow the specifications and be verifiable by an expert (see A6) in field. The trends in image quality metric (see IM2) are more important the metric values themselves.

- NFR2: **Usability** The user should be able to intuitively use the software and quickly understand what is being displayed. The software should be user-friendly, straight forward to use, and require little to no setup (see [de Fourestier \(2023\)](#)). Although the intended use is more of a qualitative nature, the user should be able to grasp any trends in the change of the image quality metric (see IM2) when the input parameters are changed. The software should have a simple user interface and be responsive when given a relatively small input image (see [input data constraints](#)). A user survey may be conducted to ascertain the software’s usability.
- NFR3: **Maintainability** The code should be clear and understandable for further development by other programmers with little to no prior experience with this software. Adding further features and extending the software should not prove to be a daunting task.
- NFR4: **Portability** The software should be cross-platform (Windows, Linux, MacOS) with little to no setup required. This can be in the form of a web-application in an HTML5 compliant web-browser.

6 Likely Changes

Here are changes listed that will likely be implemented as the software is improved.

- LC1: Give a sense of scale in real world units such as nm. The user has to provide the physical dimension of the input image.
- LC2: Simulate basic noise (such as Gaussian or Poisson) at an intensity defined by the user.
- LC3: Provide the choice of different image quality metric algorithms.

7 Unlikely Changes

- UC1: Processing multi-spectrum or multichannel images.
- UC2: Simulate electron beam physics, collision cascades, sample nature, topography, or electron-sample interactions.

8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an “X” may have to be modified as well. Table 5 shows the dependencies of theoretical models, general definitions,

data definitions, and instance models with each other. Table 6 shows the dependencies of instance models, requirements, and data constraints on each other. Table 4 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

| | A1 | A2 | A3 | A4 | A5 | A6 | A7 |
|-----|----|----|----|----|----|----|----|
| TM1 | | | X | | | | |
| TM2 | | | | | X | | |
| TM3 | | | | X | | | |
| TM4 | | | | | | | X |
| GD1 | | | | | | X | |
| DD1 | | X | X | | X | | |
| DD2 | | | | | | X | |
| IM1 | | | | | | | |
| IM2 | | | | X | | | |
| LC1 | | | | | | | |
| LC2 | | | | | | | |
| LC3 | | | | | | | |
| UC1 | | | | X | | | |
| UC2 | X | | | | | | |

Table 4: Traceability Matrix Showing the Connections Between Assumptions and Other Items

9 Values of Auxiliary Constants

This is not applicable as there no auxiliary constants defined.

| | TM1 | TM2 | TM3 | TM4 | GD1 | DD1 | DD2 | IM1 | IM2 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| TM1 | | | | | | | | | |
| TM2 | | | | | | | | | |
| TM3 | | | | | | | | | |
| TM4 | | | | | X | | | | |
| GD1 | | | | | | | | | |
| DD1 | | | | | | | X | | |
| DD2 | | | | | | | | X | |
| IM1 | | | | | | | X | | |
| IM2 | | | | | | | | | |

Table 5: Traceability Matrix Showing the Connections Between Items of Different Sections

| | IM1 | IM2 | R1 | R2 | R3 | R4 | R5 | R6 | R7 | NFR1 | NFR2 | NFR3 | NFR4 |
|------|-----|-----|----|----|----|----|----|----|----|------|------|------|------|
| IM1 | | | | | | | | | | | | | |
| IM2 | | | | | | | | | X | X | X | | |
| R1 | | | | | | | | | | | | | |
| R2 | | | | | | | | | | | | | |
| R3 | | | | | | | | | | | | | |
| R4 | | | | | | | | | | | | | |
| R5 | | | | | | | | | | | | | |
| R6 | X | | | | | | | | | | | | |
| R7 | X | | | | | | | | | | | | |
| NFR1 | | | | | | | | | | | | | |
| NFR2 | | | | | | | | | | | | | |
| NFR3 | | | | | | | | | | | | | |
| NFR4 | | | | | | | | | | | | | |

Table 6: Traceability Matrix Showing the Connections Between Requirements and Instance Models

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10 Appendix

The following is background information and some additional assumptions that are not technically required for the implementation and instance models.

1. The sample surface is flat (meaning no topography).
2. The sample surface is conductive (meaning no charge build up from electrons).
3. The beam intensity or current is considered uniform throughout the beam.
4. The beam is orthogonal to the sample surface.
5. The SEM is within a controlled environment: climate controlled and low vibration.