4D-STEM Mega Navigator (v0.1.0) - User Manual

Chapter 1 - Opening a Dataset

This application is designed exclusively for 4D-STEM datasets. Your data must be a 4D array with structure: (Ny, Nx, Qy, Qx)

Where Ny, Nx are scan (navigation) dimensions and Qy, Qx are diffraction pattern dimensions.

Anything that is not strictly 4D will fail to load. The program does not guess missing axes or reshape ambiguous data.

1.1 Opening a New Dataset

Step-by-Step (for Zarr datasets see section 1.2.3):

1. Click Open ... (top-left corner). 1
2. Navigate to your dataset.
3. Select the dataset.
4. Confirm.

During loading:

- The Load progress bar shows progress.
- The full dataset path is displayed next to it. 1A
- When loading completes, the NAV image 18 is built and the DP panel 19 displays the diffraction pattern at position (0,0).
- NAV mode defaults to VBF.

1.2 Supported File Formats

1.2.1 NumPy Compressed - .npz

The archive must contain a 4D array.

Accepted keys: data, dp, datacube, or the first available array.

Valid shapes: (Ny, Nx, Qy, Qx) or (Qy, Qx, Ny, Nx).

If axes are reversed, they are automatically transposed.

1.2.2 NumPy Array - .npy

Must contain a 4D array.

Same dimensional rules as .npz.

Memory-mapped loading is used when possible.

1.2.3 Zarr Dataset - xxx.zarr folder

Zarr is folder-based, not a single file.

You must open the entire .zarr directory, not files inside it.

How to Open a Zarr Folder

1. Click Open…
2. Navigate to the directory containing your_dataset.zarr folder.
3. Click Cancel.
4. Single-click the .zarr folder.
5. Click Open.

1.2.4 Nanomegas Blockfile - .blo

Loaded via RosettaSciIO blockfile reader. Must contain a valid 4D dataset.

1.2.5 Dectris Arina - .h5

Choose the _master.h5 file.

1.2.6 Merlin MIB Files - .mib

MIB files are not opened directly. Use the File Converters tab (see section 7.2) and convert MIB to Zarr before opening.

1.3 Automatic Shape Normalization

If dataset shape is (Qy, Qx, Ny, Nx), it is automatically converted to (Ny, Nx, Qy, Qx). If the shape is ambiguous, loading stops with an error.

1.4 What Is Not Supported

Not supported: 2D images, 3D stacks, TIFF stacks, generic HDF5, arbitrary HyperSpy files. This application is strictly for 4D-STEM datacubes.

1.5 After Opening a Dataset

NAV mode defaults to VBF.

Position (0,0) is selected.

The DP panel shows the first diffraction pattern.

You may then switch NAV modes, adjust colormaps, apply filters, compute COM/DPC/iDPC, and rebuild NAV.

Chapter 2 - Understanding the NAV Panel

The NAV panel is the navigation image of your 4D-STEM dataset.

It reduces each diffraction pattern into a single scalar value and displays it as a 2D scan image:

$$I_{\mathrm{NAV}}(y, x) = \sum_{q_y, q_x} W(q_y, q_x)\, I(y, x, q_y, q_x)$$

Where:

- $I(y, x, q_y, q_x)$is the 4D dataset
- $W(q_y, q_x)$is the selected virtual detector mask

Different NAV modes define different weighting functions W.

2.1 NAV Layout Overview

The NAV panel includes:

- The NAV image (left panel)
- A selection rectangle indicating the current probe position
- Optional overlays (rings, disks, grids, CB markers)
- Colorbar and colormap controls
- Zoom tools

2.2 NAV Modes

2.2.1 VBF Mode (Virtual Bright Field)

Uses an annular mask defined by inner and outer radii. Displays low-angle scattering contrast and thickness variations.

VBF builds NAV using an annular mask: $W(q) = \begin{cases} 1 & r_{\mathrm{in}} \le r \le r_{\mathrm{out}} \\ 0 & \text{otherwise} \end{cases}$

You control:

- Inner radius
- Outer radius
- Center offset (cx, cy)

What It Shows

- Low-angle scattering contrast
- Thickness variations
- Strain-sensitive contrast (depending on ring selection)

2.2.2 Bragg Mode

Uses one or more circular disks in reciprocal space. Useful for orientation contrast and grain mapping.

NAV is built from one or more circular disks: $W(q) = \begin{cases} 1 & (q - q_i)^2 \leq r_i^2 \\ 0 & \text{otherwise} \end{cases}$

Each disk has:

- Center (cx, cy)
- Radius
- On/Off toggle

What It Shows

- Orientation contrast
- Domain contrast
- Grain mapping signals
- Diffraction intensity tracking

2.2.3 BraggGrid Mode

Generates a periodic grid of diffraction disks based on g1 and g2 vectors. Useful for lattice-based contrast analysis.

BraggGrid builds a periodic lattice of disks: $\mathbf{q}_{nm} = \mathbf{q}_0 + n\mathbf{g}_1 + m\mathbf{g}_2$

Parameters:

- Center
- $\mathbf{g}_1, \mathbf{g}_2$
- Number of repetitions n_u, n_v

- Disk radius
- Include center toggle
- Mirror toggle

What It Shows

- Crystallographic lattice intensity
- Symmetry-based contrast
- Reciprocal lattice tracking

2.2.4 SUM Mode

Integrates total diffraction intensity per probe position.

Simple integration: $I_{\mathrm{NAV}}(y,x) = \sum_{q_y,q_x} I(y,x,q_y,q_x)$

What It Shows

- Total scattered intensity
- Thickness contrast
- Mass-thickness mapping

2.2.5 MAX Mode

Displays the maximum diffraction intensity per probe position.

Maximum projection: $I_{\mathrm{NAV}}(y,x) = \max_{q_y,q_x} I(y,x,q_y,q_x)$

What It Shows

- Strongest diffraction event per probe
- Useful for detecting sharp reflections

2.3 Rebuild NAV

Changing NAV parameters marks the image as dirty. You must press 'Rebuild NAV' to update the image. Rebuild can be full or visible-only if zoomed.

2.4 Clicking in NAV

Clicking inside NAV updates the DP panel and moves the selection rectangle.

2.5 Zooming NAV

Use 'Zoom NAV' to draw a rectangle and zoom. Use 'Reset Zoom' to restore full view. Zoom affects display only, not data.

2.6 NAV Display Controls

You can change colormap, reverse it, save NAV image, and adjust nm/px calibration. Calibration affects only axis display, not data values.

2.7 Log Scaling

Applies log(1 + I) to improve visibility of weak signals. Affects display only.

2.8 Center-of-Beam (CB) Anchors

Allows manual correction of scan-dependent beam shifts. CB anchors can be added, cleared, and used during NAV rebuild.

2.9 COM Overlay

If COM is computed, vector arrows can be overlaid on NAV. Arrows represent beam deflection direction.

2.10 Performance Considerations

For large datasets:

- Zoom before rebuilding
- Use visible-only rebuild

2.11 Expand / Collapse Control Tabs

A red triangle button 28 allows collapsing the tab controls. When collapsed, NAV and DP plots expand vertically. Collapsing does not modify data or trigger Rebuild. Expanding restores the controls without recalculation.

Chapter 3 - Understanding the DP Panel

The DP panel displays the diffraction pattern at the currently selected scan position.

If the selected probe position is (y, x), the DP panel shows $DP(q_y, q_x) = I(y, x, q_y, q_x)$.

This is a direct slice of the 4D dataset.

3.1 DP Panel Layout

The DP panel includes:

- Diffraction image
- Colorbar
- Optional overlays (VBF rings, Bragg disks, BraggGrid, CB crosshair, COM arrow)
- Colormap controls
- Axis calibration (nm^-1/px)

3.2 Updating the DP

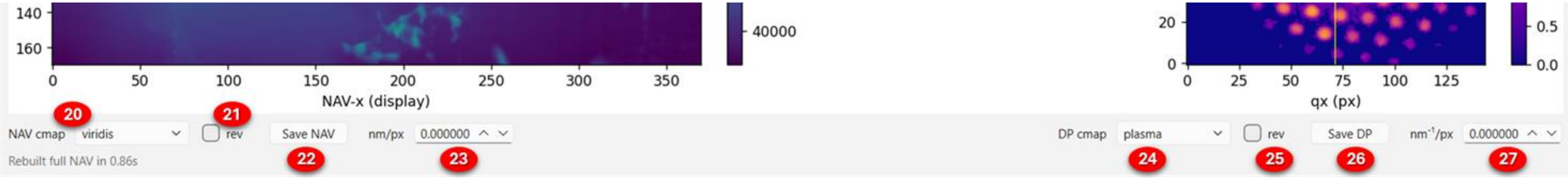
The DP updates automatically when clicking in NAV or moving with keyboard arrows. No rebuild button is required for DP updates.

3.3 Log Scaling

If log is enabled, the display uses $I_{\text{disp}} = \log(1 + I)$ .Log scaling affects display only, not computation.

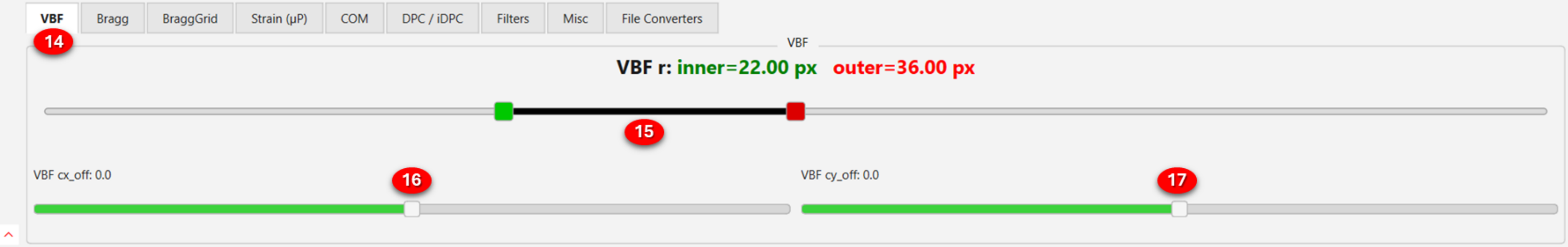
3.4 DP Display Controls

You can change colormap, reverse it, save the DP image, and adjust axis calibration. Calibration changes axis labels only.



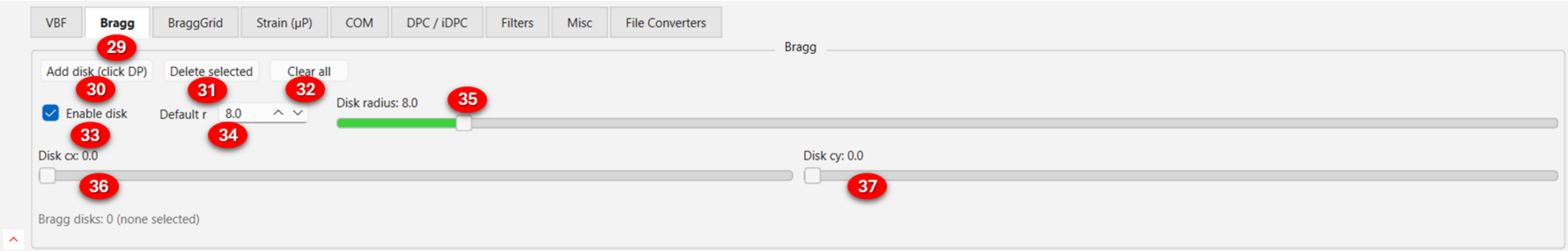
3.5 VBF Overlay

Inner and outer rings (15) indicate the annular mask used for NAV. Overlay updates instantly when parameters change.



3.6 Bragg Disk Overlay

Active Bragg disks are shown as circles on the DP image. Disk positions match NAV settings.



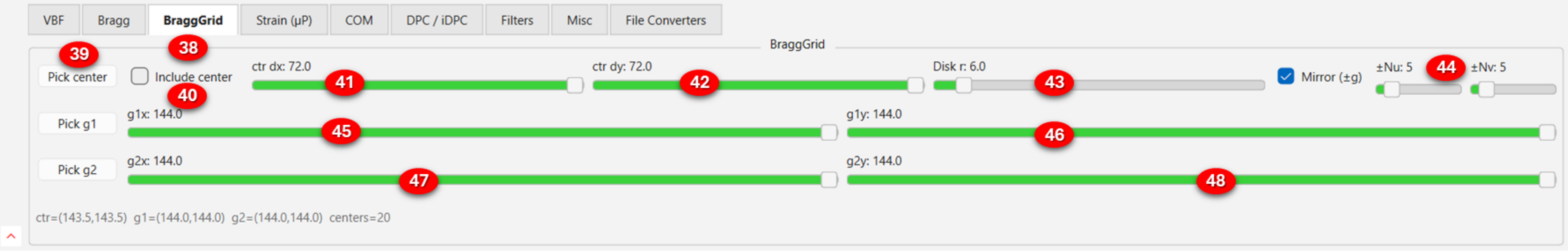
In Bragg mode:

- Each active disk is drawn as a circle.
- Disk center and radius match NAV parameters.
- Disks can be enabled/disabled individually.

The overlay allows precise positioning before rebuilding NAV.

3.7 BraggGrid Overlay

Displays a lattice of disks defined by reciprocal vectors g_1 and g_2. Mirror and center options modify the grid pattern.



In BraggGrid mode a lattice of disks is drawn. Defined by: $\mathbf{q}_{nm} = \mathbf{q}_0 + n\mathbf{g}_1 + m\mathbf{g}_2$ Where:

- $\mathbf{q}_0$ is the center
- $\mathbf{g}_1, \mathbf{g}_2$ are reciprocal lattice vectors
- $\boldsymbol{n}, \boldsymbol{m}$ are repetition indices

Mirroring and center inclusion options modify the disk pattern.

3.8 Center-of-Beam (CB) Crosshair

Shows the current beam center if CB correction is active. DP centering affects display only.

3.9 COM Arrow Overlay

If COM is computed, a vector arrow indicates beam deflection. Deflection is defined as shift from reference center.

A vector arrow is drawn: $\vec{D}(y,x) = (\Delta q_x, \Delta q_y)$ Where: $\Delta q_x = \langle q_x \rangle - q_{x0}$ & $\Delta q_y = \langle q_y \rangle - q_{y0}$

This represents beam deflection at that probe position.

3.10 DPC and iDPC Relation

DP always displays the raw diffraction pattern. DPC and iDPC calculations do not modify DP display.

3.11 Keyboard Control

Arrow keys move the probe position.

Focus determines whether NAV or DP captures arrow control.

3.12 Saving the DP

Press Save DP to export the currently displayed diffraction pattern.

Export includes current display settings.

3.13 What the DP Panel Is - and Is Not

DP panel is a raw diffraction slice from the 4D dataset.

It is not a reconstructed image or phase map.

Chapter 4 - Strain (μProbe) Analysis

4.1 Overview

The strain module computes lattice strain maps from tracked Bragg reflections across the scan.

At each scan position:

1. Bragg vectors are measured in reciprocal space.
2. They are compared to a reference configuration.
3. A local deformation gradient tensor F is fitted.
4. Strain and rotation are extracted.

The method is based on reciprocal-space vector mapping: $g_{\exp} \approx F \cdot g_{ref}$

4.2 Reference and Experimental g-Vectors

For each selected reflection k:

$$g_k^{ref} = \begin{bmatrix} g_{(x,k)}^{ref} \\ g_{(y,k)}^{ref} \end{bmatrix}$$

$$g_k^{\exp} = \begin{bmatrix} g_{\{x,k\}}^{\exp} \\ g_{\{y,k\}}^{\exp} \end{bmatrix}$$

Vectors are measured relative to the local central-beam (CB) center.

Experimental positions are determined via:

- Cross-correlation patch matching
- Subpixel peak refinement
- Optional bandpass filtering

4.3 Patch Extraction and Cross-Correlation

Each Bragg disk is tracked using a square patch of size: $(2h + 1) \times (2h + 1)$ Where **Half patch (*h*)** controls spatial support.

The shift between reference and experimental patch is determined by FFT phase correlation: $\Delta g_k = g_k^{\exp} - g_k^{ref}$

Subpixel refinement is performed using quadratic interpolation.

4.4 Weighted Least Squares Fit of F

The deformation gradient is obtained by minimizing: $\sum_{\mathrm{k}} w_{\mathrm{k}} \left\| g_k^{\exp} \text{-F} g_k^{ref} \right\|^2$ Weights follow: $w_k = q_k^p$

4.5 Strain Tensor Extraction

From: $\mathrm{F} = \begin{bmatrix} \mathrm{F}_{00} & \mathrm{F}_{01} \\ \mathrm{F}_{10} & \mathrm{F}_{11} \end{bmatrix}$

Small-strain approximation: $\varepsilon = \frac{1}{2}(F + F^T) - I$

Components: $\varepsilon_{xx} = F_{00} - 1$; $\varepsilon_{yy} = F_{11} - 1$; $\varepsilon_{xy} = \frac{1}{2}(F_{01} + F_{10})$

Rotation: $\theta = \frac{1}{2}(F_{10} - F_{01})$

4.6 Key Parameters (Practical Meaning)

- **Half patch**: tracking window size (typical microprobe: 12–25 px)
- **qmin**: minimum correlation quality (typical: 0.2–0.4)
- **shift max**: maximum allowed shift in pixels (typical: 3–6 px)
- **weight power**: weighting strength (typical: 1–2)
- **min used spots**: minimum valid reflections per pixel (typical: 3–5)

4.7 Output Maps

The module outputs 2D maps (Ny, Nx) for:

- ε_{xx}, ε_{yy}, ε_{xy}
- rotation θ
- used-spot count
- residual / fit error

4.8 Filtering Options

Optional bandpass filtering may be applied: $I' = G_{\{\sigma_{lo}\}(I)} - G_{\{\sigma_{hi}\}(I)}$

This helps suppress background and high-frequency noise for more stable correlation.

4.9 Recommended Workflow

1. Define reflections (BraggGrid or manual Bragg disks).
2. elect a reference region / reference g-vectors.
3. Tune Half patch, qmin, shift max.
4. Compute strain.
5. Inspect used-spot count + residual maps.
6. Refine parameters if needed.

4.10 Stability Notes

Unstable strain usually comes from too few reflections, poor CB centering, overlapping disks, excessive noise, or an overly large shift_max. If reflections are nearly collinear, the fit becomes ill-conditioned.

Chapter 5 - COM, DPC and iDPC Analysis

This chapter explains COM (Center of Mass), DPC (Differential Phase Contrast), and iDPC (Integrated DPC) analysis. All are derived from diffraction pattern intensity shifts.

5.1 Physical Background

Electron phase shift: $\phi(x, y) = \sigma V(x, y)t$

Where:

- σ = interaction constant
- $V(x, y)$ = projected potential
- t = thickness

The phase gradient causes beam deflection: $\Delta\mathbf{q}(x, y) \propto \nabla\phi(x, y)$

COM and DPC measure this deflection.

iDPC integrates it back into a potential-like image.

5.2 Center of Mass (COM)

COM is computed from intensity-weighted averages of q_x and q_y.

Deflection maps are defined relative to a reference beam center.

5.3 DPC (Differential Phase Contrast)

In this implementation, DPC is equivalent to COM shift. The magnitude is: $|DPC| = \sqrt{\mathrm{D}_x^2 + \mathrm{D}_y^2}$

5.4 CB Correction Options

Global offset removal subtracts mean deflection. Removes global detector mis-centering.

Gaussian drift removal subtracts low-frequency background. Removes slow scan-coil distortions.

5.5 iDPC (Integrated DPC)

iDPC reconstructs a scalar image from the DPC vector field.

Given $\nabla\phi = (D_x, D_y)$ The reconstructed phase is obtained by solving: $\nabla^2\phi = \nabla \cdot D$

It solves a Poisson equation in Fourier space: $\phi(k) = \frac{ik_x D_x(k) + ik_y D_y(k)}{k_x^2 + k_y^2}$

Zero-frequency component is set to zero.

What iDPC Shows:

- Projected electrostatic potential
- Atomic columns
- Light element contrast
- Thickness-sensitive features

Unlike raw DPC, iDPC produces a scalar image.

5.6 Step Size and Subsampling

COM/DPC can be computed with adjustable step size.

This reduces computation:

- Step = 1 → full resolution
- Step = 2 → every second probe
- Larger step → faster but lower resolution

5.7 Masking Options

Optional VBF mask can be applied during COM computation.

Reduces high-angle noise, Inelastic background and detector edge artifacts.

5.8 Display in GUI

NAV can display Dx, Dy, magnitude, or iDPC reconstruction. DP panel remains unchanged.

Optional quiver arrows can overlay vector field or color-coded magnitude.

5.9 Performance Considerations

Computation scales with Ny * Nx * Qy * Qx. O(NyNxQyQx)

Use subsampling for large datasets.

5.10 What These Methods Are - and Are Not

They measure phase gradients, probe deflection and approximate electrostatic field mapping tools.

They are not absolute potential maps without calibration.

Chapter 6 - Filters and Image Processing

This chapter explains how filtering is implemented in the GUI and how it affects NAV display, DP display, and COM/DPC computation. Filters are applied at the display level unless explicitly stated. Raw 4D data is not modified.

6.1 Filtering Philosophy

Filtering improves visibility, suppresses noise, and stabilizes COM/DPC computation. Filtered data is computed as $I_{filtered} = F(I)$.

6.2 NAV Filters

NAV filters operate on the 2D navigation image.

Available filters include: None, Gaussian, Uniform (mean), Median, Wiener (2D).

6.2.1 Gaussian Filter

Applies Gaussian smoothing controlled by sigma.

Reduces high-frequency noise while preserving low-frequency contrast.

6.2.2 Uniform (Mean) Filter

Applies box averaging over a local window.

Fast but may blur edges.

6.2.3 Median Filter

Replaces each pixel with the median value in a local window.

Effective against salt-and-pepper noise.

6.2.4 Wiener Filter (2D)

Adaptive noise-reduction filter using local mean and variance.

Useful when noise varies across the image. This implementation uses standard 2D Wiener filtering (not radial).

6.3 DP Filters

DP filtering acts on the diffraction pattern slice. Used to improve COM stability and suppress detector noise. May affect COM computation if configured to use filtered data.

6.3.1 Log Scaling vs Filtering

Log scaling uses log(1 + I) to compress dynamic range. Log affects display only, not spatial structure. Filtering modifies spatial information.

6.3.2 Radial vs 2D Filtering

Radial filtering operates in diffraction space as a function of radius.

NAV Wiener filter in this GUI is standard 2D spatial filtering.

Radial filtering is not the default NAV filter.

6.4 Filtering and COM/DPC Stability

Noise propagates into COM through intensity-weighted averages. Mild smoothing and masking can improve stability. Over-filtering reduces spatial resolution.

6.5 When to Filter

Use filtering for noisy or low-dose data. Avoid heavy filtering in quantitative or high-resolution analysis.

6.6 Saving Filtered Images

Saved NAV and DP images reflect current display settings. Raw dataset remains unchanged.

6.7 Performance Considerations

2D filtering is fast. Filtering the full 4D dataset is computationally expensive.

6.8 Summary

Filters improve visualization and stability but do not increase resolution or recover lost information. Filtering is a tool, not a correction for poor acquisition.

Chapter 7 - File Converters and Data Management

This chapter explains the built-in file converters, large dataset handling, metadata storage, and best practices for managing 4D-STEM data.

The GUI is optimized for large datasets (tens of GB).

7.1 Why File Conversion Is Necessary

Raw detector formats such as Merlin .mib are not optimized for interactive analysis. Chunked, compressed, lazy-loadable formats are required for efficient workflows. Zarr is the recommended format.

7.2 MIB → Zarr Converter

Located in the File Converters tab.

Converts .mib datasets into chunked Zarr format.

7.2.1 What It Does

1. Opens the .mib dataset.
2. Reads associated. hdr metadata (if available).
3. Determines navigation shape.
4. Creates a chunked Zarr dataset.
5. Writes compressed data.
6. Stores metadata in Zarr attributes.

7.2.2 Output Structure

Output is a folder named dataset.zarr containing .zgroup, .zattrs, and data chunks. Data is stored as (Ny, Nx, Qy, Qx).

7.2.3 Compression

Uses Blosc with Zstandard (zstd) and bitshuffle. Reduces disk usage and improves I/O performance.

7.2.4 Navigation Shape (nav_shape)

Correct navigation shape is critical for accurate scan reconstruction. Ny × Nx must equal total frames. Incorrect nav_shape leads to misaligned images and wrong analysis results.

7.2.5 Chunking Strategy

Recommended chunking: $(4,4,Q_y,Q_x)$. Small navigation tiles with full diffraction patterns per chunk. Improves NAV rebuild and COM performance.

7.2.6 Lazy Loading

Zarr datasets are opened lazily. Only accessed chunks are loaded into memory. Memory usage depends on active chunks, not total dataset size.

7.2.7 Metadata Storage

Zarr attributes store source file path, detector shape, navigation shape, HDR contents, chunk size, and compression settings. Ensures reproducibility and traceability.

7.2.8 Saving NAV and DP

Saved images reflect current display settings. Raw dataset is not modified.

7.2.9 Best Practices

1. Always convert MIB to Zarr.
2. Keep original raw files archived.
3. Use meaningful dataset names.
4. Store calibration information separately.
5. Verify dataset after conversion.

7.2.10 Performance Scaling

Processing cost scales with Ny × Nx × Qy × Qx.

Use visible-only rebuild and subsampling to optimize performance.

7.2.11 System Design Scope

Optimized for 4D-STEM strain mapping, COM/DPC workflows, and interactive large dataset analysis. Not intended for small 2D TEM image processing.

Chapter 8 - Advanced Usage and Expert Workflow

This chapter describes advanced strategies for performance optimization, stability, and physically meaningful analysis. These guidelines are intended for experienced users working with large 4D-STEM datasets.

8.1 Efficient Large-Dataset Workflow

Recommended steps:

1. Convert MIB to Zarr.
2. Zoom into region of interest.
3. Use visible-only rebuild.
4. Increase COM step size during exploration.
5. Switch to full resolution for final computation.

Processing cost scales with Ny × Nx × Qy × Qx.

8.2 Using CB Anchors Properly

Add anchors across the scan area (at least four quadrants).

Build CB map and enable 'Use CB map (NAV rebuild)'.

CB correction shifts masks tile-wise to compensate beam drift.

Verify physical consistency after correction.

8.3 Choosing the Right NAV Mode

- Thickness contrast → SUM or low-angle VBF.
- Strain or domain contrast → Bragg or BraggGrid.
- Orientation mapping → BraggGrid.
- Beam deflection or fields → COM / DPC.

No single mode is universally correct.

8.4 COM / DPC Best Practices

1. Use annular masking before COM to suppress noise.
2. Remove global offset unless absolute calibration is known.
3. Remove low-frequency drift carefully without over-smoothing.

8.5 iDPC Reconstruction Tips

iDPC solves a Poisson equation in Fourier space.

Zero-frequency component is undefined; absolute offset is arbitrary.

Remove global offset and drift before integration.

Avoid aggressive smoothing before reconstruction.

8.6 Grid-Based Bragg Analysis Strategy

Set accurate center and reciprocal vectors (g1, g2).

Start with small disk radius and increase gradually.

Avoid disk overlap to prevent artificial contrast.

Use mirror option only when symmetry requires it.

8.7 Performance Tuning

If GUI feels slow:

- Collapse tabs.
- Reduce COM resolution.
- Avoid unnecessary full rebuilds.
- Disable overlays when not needed.

8.8 Avoiding Common Expert Mistakes

Over-filtering reduces spatial resolution.

MAX mode is qualitative only.

Detector calibration is required for physical units.

Always verify raw DP before drawing conclusions.

8.9 Interpreting COM/DPC Physically

Beam deflection relates to projected electric field.

Magnetic and thickness contributions are not separated automatically.

Interpret results carefully with physical reasoning.

8.10 Publication-Quality Workflow

1. Convert to Zarr.
2. Verify geometry and calibration.
3. Apply CB correction.
4. Compute COM at full resolution.
5. Apply minimal smoothing.
6. Perform iDPC reconstruction.
7. Document all parameters used.

8.11 Reproducible Pipelines

Record NAV mode, mask parameters, grid vectors, COM step size, CB correction, and filters used.

Reproducibility depends on parameter transparency.

8.12 Final Expert Advice

This GUI is a tool for exploration, not a black box.

Use it deliberately and combine results with sound physical reasoning.

8.13 Final Notes

This GUI is optimized for interactive 4D-STEM analysis.

Accurate physical interpretation requires correct calibration, proper masking, and careful parameter documentation.

Always verify results using raw diffraction inspection and physical reasoning.

Appendix - Reference and Troubleshooting

A. Keyboard and Interaction Shortcuts

Action	Function	Notes
Arrow Keys	Move scan position	Updates DP instantly
Click in NAV	Select scan position	Activates probe selection
Click in DP	Used when adding disks / picking g-vectors	Required for Bragg / BraggGrid
Click Control Title	Reset parameter to default	Works for NAV and Strain controls
Zoom NAV	Enable zoom selection	Drag rectangle to define region
Reset Zoom	Restore full NAV view	Does not rebuild NAV
Rebuild NAV	Recompute NAV image	Required after parameter changes
Collapse Tabs	Hide control panels	Layout only
Help → Manual / Website	Open documentation links	No computation

B. Parameter Reference

B.1 NAV Parameters

Parameter	Location	Effect	Physical Meaning
VBF inner / outer radius	VBF tab	Defines annular mask	Scattering angle range
Bragg disk radius	Bragg tab	Defines disk integration area	Specific reflections
g1, g2 vectors	BraggGrid tab	Defines lattice periodicity	Reciprocal lattice basis
±Nu / ±Nv	BraggGrid tab	Grid repetitions	Number of reflections used
Include center	BraggGrid tab	Adds central beam	Optional reference
Use CB map (NAV rebuild)	NAV	Applies spatial CB shift	Drift correction
Visible-only rebuild	Zoomed NAV	Rebuilds zoom region only	Performance optimization
Rebuild NAV	Top panel	Recomputes NAV image	Applies mask to 4D data

B.2 Strain Parameters

Parameter	Effect	Recommendation
Half patch	Bragg tracking window size	12–25 px (microprobe)
qmin	Minimum correlation quality	0.2–0.4
shift max	Max allowed spot shift	3–6 px
weight power	Emphasizes good reflections	1–2
min used spots	Minimum reflections per pixel	≥3

Bandpass (sigma lo/hi)	Improves cross-correlation	Mild filtering
Reference region	Defines undeformed lattice	Choose stable area

B.3 COM / DPC Parameters

Parameter	Effect	Recommendation
COM step size	Controls spatial resolution	Use >1 during exploration
Global offset removal	Subtracts mean deflection	Enable unless absolute calibration needed
Drift removal (Gaussian)	Removes low-frequency background	Use moderate sigma
VBF mask in COM	Suppresses high-angle noise	Recommended for noisy data
iDPC integration	Reconstructs scalar potential-like map	Use full-resolution COM input

C. CB Map Controls

- Add CB anchor: Stores local CB shift
- Show anchors: Visual overlay only
- Build CB map: Interpolates $\Delta x(y,x)$, $\Delta y(y,x)$
- Use CB map (NAV rebuild): Applies drift correction during rebuild
- DP center (CB map): Display-only stabilization

D. Troubleshooting Guide

Problem	Possible Cause	Solution
NAV does not change	Forgot Rebuild	Click Rebuild NAV
Strain noisy	Too few reflections	Increase min used spots
Strain unstable	shift_max too large	Reduce shift_max
Large strain artifacts	Poor CB centering	Build CB map
BraggGrid misaligned	Incorrect g_1/g_2	Repick center and vectors
Zarr folder not selectable	File dialog behavior	Select folder then Cancel
GUI slow	Large grid or CB map	Use visible-only rebuild
DP appears shifted	CB map active	Check DP center toggle
iDPC background strong	No drift removal	Enable Gaussian correction

E. Best Practices

- Always verify raw diffraction patterns.
- Use visible-only rebuild for tuning.
- Inspect used-spot count map in strain analysis.
- Keep shift_max physically reasonable.
- Document calibration values.
- Use CB map for large scan drift.
- Reset parameters via clickable titles when tuning becomes unstable.