

PROBE CORRECTOR WISDOM

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This document contains a collection of information about the hexapole probe corrector, as well as an alignment procedure that achieves high resolution STEM imaging in as little as 30 minutes. I also philosophize on the entire endeavor.

1. How It Works

The information in this section is based on the chapter by Krivanek in the *Handbook of Charged Particle Optics* [1]. Thus the aberrations are written in the Krivanek notation, which differs from the Haider notation used in the CEOS software and literature. The aberration $C_{m,n}$ has m th order radial dependence and n -fold azimuthal symmetry.

The CEOS probe corrector available on FEI microscopes is of the “indirect-action” type, where the correcting effect is produced by the combined effect of lower order aberrations. In the case of the hexapole-hexapole corrector, this is achieved by the combination of two “thick” hexapoles. A hexapole element primarily produces a three-fold distortion of the beam, but if the hexapole is extended along the beam direction an additional deflection is produced that amounts to a negative spherical aberration. This extra deflection is radially symmetric, and always negative.

The spherical aberration produced by a single extended hexapole of length L which primarily produces three-fold astigmatism $C_{2,3}$ is

$$C_{3,0} = \frac{-(C_{2,3})^2 L}{3f^2 M^2} \quad (1)$$

where f is the objective lens focal length and M is the magnification between the hexapole and the objective lens. ¹

¹ The magnification between the hexapoles and the objective lens is fixed in order to minimize C_5 , so the C3 button in the probe corrector software adjusts the excitation of the hexapoles.

The three-fold distortion is cancelled by passing the beam through a second hexapole element of opposite excitation² (which additionally contributes a negative spherical aberration). The beam exiting the first hexapole must be imaged into the second hexapole with high precision in order to cancel the three-fold distortion: this is accomplished by a pair of round lenses arranged in an anti-rotation doublet³. Further round lenses are required to image the source into the hexapole system and couple the beam into the objective lens.

The three-fold astigmatism produced by one of the hexapoles is on the order of 500 μm , which is perhaps 10,000 times larger than tolerable for high resolution imaging. Therefore, the required precision of the compensation by the second hexapole is very high. Miscentering of the beam through a hexapole element by a distance τf primarily induces a two-fold astigmatism⁴:

$$C_{1,2} = 2C_{2,3}\tau \quad (2)$$

For typical values in the hexapole corrector, 2 nm of $C_{1,2}$ is produced by a displacement of the beam of only 8 nm in the hexapoles. To keep two-fold astigmatism below this value, the beam in the hexapoles must be centered to a precision of 4 μrad . This high sensitivity leads to the very strong drift of two-fold astigmatism. Miscentering of the beam entering the objective lens primarily produces axial coma:

$$C_{2,1} = 3C_{3,0}\tau \quad (3)$$

This alignment is less demanding than the hexapole centering, requiring alignment on the order of 300 nm or 150 μrad .

2. Information From the CEOS Manual

The CEOS manual can be found on the microscope computer in C:\Titan\tem_help.

2.1. Manual Buttons

The actions of the Manual Correction buttons are described as follows:

- **AT_A1:** Shifts the beam between the two hexapoles
- **AT_A1fine:** Stigmates with QPol and compensates shifts with DP11

² Or, equivalently, by imaging it with magnification of -1 into a second hexapole of equal excitation.

³ Round lenses produce a Larmor rotation of the beam, which can be cancelled with a pair of lenses.

⁴ The “A1 coarse” button in the probe corrector software controls this shift. The “A1 fine” is a conventional quadrupole stigmator.

- **AT_A2:** Changes main hexapoles and transfer lenses
- **AT_A2fine:** Changes the hexapole stigmator HPol (a weak, short hexapole at the midplane between the main hexapoles)
- **AT_B2:** Tilts beam in the main hexapoles, with other elements involved to compensate A1 and shift
- **AT_B2fine:** Tilts the beam in the upper objective
- **UserBeamShift:** Uses the beam tilt Btlt and Bsh coils at the entrance of the corrector. (I believe this shift compensates for A1 and B2.)
- **BeamTilt:** (this is the same as **WD**)

2.2. Corrector Elements

A schematic of the S-CORR corrector is shown in Figure 1.

Some of the deflectors and stigmators that are shown in the corrector software and optical diagrams are actually part of the base microscope. Element DP12 is virtual and realized via DC offsets applied to the STEM scan coils.

2.3. CEOS Recommendations

- Tuning should be performed with a probe current of 120-200 pA. With longer exposure times for the images, tuning is possible with as little as 30 pA.
- Fifth order aberrations are stable over long time periods, and not user-alignable. Fourth-order aberrations are stable over “many weeks.” Third order aberrations are stable for days, and should not be adjusted until second order aberrations are corrected.

2.3.1. Achievable Values

Aberration	Limit
A1	5 nm
B2	50 nm
A2	100 nm
C3	2 μm
A3	1 μm
S3	700 nm
A4	10 μm

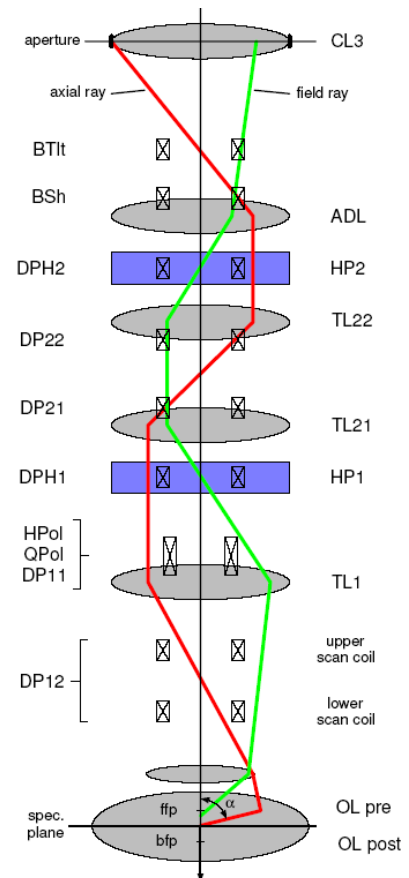


Figure 1. Optical system of the S-CORR corrector. The axial ray crosses the optic axis at locations where a demagnified image of the source is present.

B4	10 μm
D4	4 μm

3. Alignment Procedure

This is a highly abbreviated description of the alignment procedure, meant for experienced users. It is assumed that the user is already familiar with the proper alignment of each individual control, except in cases where there is a noteworthy deviation from a “standard” alignment routine. In particular, it is assumed that the user is able to diagnose the first and second order aberrations of the system from the Ronchigram. If adjustment of the sample plane is not necessary, these steps can often be completed in under 30 minutes.

3.1. Initial TEM Alignments

TEM alignments are largely optional. If the microscope is already in STEM when you arrive, it’s probably better to just leave it in STEM rather than disturb the lenses to do the TEM alignments. All but one of these alignments are available in STEM mode, and so it is better to do those after switching into STEM. Only **Beam Tilt p-p** is not possible in STEM⁵, so every other alignment in the following block is being done simply to get a reasonable enough looking beam to set the pivot points well. Should you choose to perform TEM alignments, follow these steps. However, feel free to skip these alignments.

1. Use Microprobe TEM, 3 condenser mode
2. Center the C2 aperture using the **Center C2 Aperture** direct alignment at around 20kx magnification
3. Use **Condenser Center TEM** direct alignment at around 20 kx magnification
4. Use **Beam Shift** direct alignment and **Condenser Stigmator** as needed
5. Align **Beam Tilt p-p** at the highest SA magnification

3.2. Ancillary Alignments

If you need to perform a gain reference on one of the detectors, or any other similar alignment that has particular requirements

⁵ This pivot point is likely not important for STEM, since the corrector tilt pivot point is the critical one to manage, and its impurity is managed within the calibrated correction buttons.

on the beam, now is the time to do that. If you wait until later you may have to redo many critical alignments if you need to change spot size or gun lens to get enough current.

3.3. Rough STEM Alignments

The following alignments can be conducted over vacuum or with a sample in the beam path.

1. In the probe corrector UI, locate the “Exported Elements” tab and ensure all *stigmator* values here are zero. If there are nonzero values, these can be cleared by resetting the stigmators in the microscope UI. Some elements related to the transfer or adapter lenses (TL/ADL) may be nonzero and this is okay.
2. Go out of **Diffraction** and retract the HAADF detector
3. Use **Beam Shift** direct alignment to center the beam at moderate (100 kx) magnification
4. Perform **Center C2 Aperture** direct alignment at around 20 kx magnification
5. Perform **Condenser Center STEM** direct alignment, also at around 20 kx magnification⁶
6. Finally, center the beam with **Beam Shift** direct alignment at the highest SA magnification
7. Perform **Beam Tilt** direct alignment at the highest SA magnification to set the fine tilt of the beam.
8. Return to **Diffraction**

⁶ This adjusts the tilt of the beam in the C2/C3 zoom system, and so is important if you will later vary the convergence angle or spot size.

3.4. Specimen Positioning

The height of the sample in the objective lens is critical to the alignment of the probe corrector. Locating the “sweet spot” is often challenging. There are two approaches that seem to work well enough:

3.4.1. Using a known reference:

When using a factory alignment file (without loading a FEG register) and the same spot size (generally spot 6) and convergence angle (generally 30 mrad) as the factory alignment, the probe crossover is generally already at the correct location.

- Using these optical settings, bring the sample into focus using the Z height control.

- If other optical settings are desired, change the spot size or convergence angle after moving to this reference height, then bring the image into focus using **Intensity List (FOCUS)** direct alignment.

3.4.2. Locating the corrector pivot point

The most important consequence of using the wrong specimen height during correction⁶ is that the image shift induced by the beam tilt used for tableau measurements will be unacceptably large. Therefore, we locate the appropriate height by finding the position that minimizes image shift upon tilting.

- Bring the sample approximately into focus using the Z height
- Make sure the controls are configured so that the Focus knob controls the Objective lens and the Intensity knob controls the C3 lens (“Intensity & Objective” in the STEM Focus control flap-out)
- Open the **Manual Correction** tab of the probe corrector GUI and select **Beam Tilt** with the bit multiplier set so that one click yields 10-20 mrad tilt
- Start a STEM search with a fast dwell time (100 ns)
- Apply one click of **Beam Tilt**. The image will shift as a result.
- Use the Z height to try to align the shifted image with its old location. If the image is out of focus, adjust the focus with **Intensity** knob.
- Continue adjusting Z height and **Intensity** focus until rocking the beam tilt by one click does not move the image by more than a few nanometers. (Note that if you pass the “sweet spot”, the direction of the image shift will flip, i.e. if a +10 mrad tilt used to move the image left but now moves the image right, you have gone past the sweet spot). You will likely need to use STEM magnification of around 600 kx or more to reach the necessary precision.
- Once the image no longer shifts when tilting the beam, use **Intensity List (FOCUS)** direct alignment to focus the image.

⁶ This is the most immediately obvious consequence of being at the wrong height, but the setting of the sample height is also important for minimizing the C_5 of the system. It appears, from experience, that this is indeed the C_5 -minimizing height. I’ve witnessed the system being tuned with 4 μm of objective defocus set, and with the sample at that focal point the aberration measurement reported about 1 mm of C_5 . At the proper height, the C_5 is always below the measurement error.

3.5. STEM Hand-Tuning

It is **critical** that you **never use a beam position marker** during hand tuning of the Ronchigram. You **must** ensure that

the beam is centered on the optic axis during tuning, as large offsets of the beam position induce off-axial aberrations (notably B2). The following steps should all be conducted with the STEM magnification set to at least 225 kx (and preferably 1 Mx or more), as there is a shift of the beam center position with lower magnifications.

1. Find a suitable region of the tuning grid. Use only a completely intact square on the grid.
2. Now that the height of the source image at the entrance of the corrector has been defined, only bring the sample into focus using the Z height control. At this point, this should generally be possible using only the piezo controls.
3. Record the position of the C2 aperture by drawing a circle around the Ronchigram on the flu-cam
4. Choose the largest C2 aperture, and roughly center it (exact centering is not critical)
5. You will likely need to retract the HAADF in order to observe the full Ronchigram
6. Maximize the Ronchigram magnification in the central region using the piezo Z control
7. Use the **Probe A1** stigmator control *in the microscope UI* to adjust stigmatism as well as possible
8. Use the **Probe B2** stigmator control *in the microscope UI* to minimize B2. This is observable as a lack of side-to-side motion of the Ronchigram sweet spot as the focus is wobbled. The Ronchigram should expand concentrically from a single point, which is hopefully (but not necessarily) at the center of the Ronchigram.
9. Bring the sample into best focus using the piezo Z
10. Iterate **Probe A1**, **Probe B2**, and Z height controls once or twice, until the Ronchigram is as flat as possible. This degree of tuning is generally sufficient to reach $<1 \text{ \AA}$ resolution at 300 kV.
11. If it is impossible to improve the B2 to an acceptable level, the most likely culprit is that the beam has shifted far off-axis. Go out of Diffraction and use **Beam Shift** to bring it back to the center.
- 12.

The primary consequences of the beam not being centered within each corrector element and the upper objective are strong A1 and B2 (this is inherent to the design of the system). The tuning of A1 and B2 at this initial stage ultimately amounts to *centering* the beam through various corrector elements and the upper objective: the coarse controls for these aberrations are *shifts* (at different layers) rather than *stigmation*. Thus if large corrections are needed, the impurity of the coarse controls can mean that iteration between **A1**, **B2**, and **Beam Shift** are necessary. For this same reason, *do not use the **Condenser Stigmator** at this stage*, as it is critical to get the beam centered in order for higher-order tuning to succeed: the stigmator can null the A1 induced by off-centering but not the higher order combination aberrations, and has additional side effects (see Section 3.6.3)

13. Return to the original C2 aperture size, and center it on the marker used earlier.
14. If you intend to do EELS, now you may adjust the appearance of the probe in real space by going out of **Diffraction** and using the **Objective Stigmator** to make the beam round. After doing this, double check the A1 and B2 after returning to **Diffraction** and correct any errors induced by switching out of **Diffraction**.

3.6. Probe Corrector Auto-Alignment

Once the system is hand-tuned to the point that A1, B2, and the beam shift are moderately well aligned, we proceed to use the auto-alignment tools for checking and correction of the higher order aberrations. Once we begin this process, it is generally best to avoid going out of Diffraction. The previous steps should have set the overall beam path through the corrector to be reasonably well centered, and you should not manually adjust it any further. The auto-alignment tools have reasonably good purity for managing these shifts, as long as your starting point is good.

During the aberration measurements, watch the images for signs of contamination. If a large carpet of carbon builds up, or if the grid falls apart, you will have to move to a new location and wait a minute or two for the stage to settle.

1. The auto-correction tools require a particular setup of STEM image. Set the camera length for an inner collection angle of 45-50 mrad (for a 30 mrad convergence angle); this is shorter than traditional for true HAADF con-

trast, but here it seems more useful to have greater signal than true HAADF contrast. It is very important to set the bias and gain of the HAADF amplifier correctly:

- Start searching, and bring up the Scope tool. Connect **Brightness** and **Contrast** to the MF knobs.
 - Blank the beam. Use **Brightness** to bring the dark level *just* above zero counts.
 - Unblank the beam. Scan at 450 kx or so, with a well focused image. Use **Contrast** to bring the white level *just* up to saturation, or even slightly beyond. Some clipping of the high values is acceptable.
2. Set the STEM magnification to 225-350 kx.

3.6.1. Low Orders

1. In the probe corrector software, go to the **C1A1** tab, and press Start. The system will now acquire Gaussian-, under- and over-focused images of the area and estimate the 0th through 2nd order aberrations. In this view, the goal is to make every aberration appear colored white; yellow-orange-red indicates aberrations too large for good imaging. *If the measurement lines are grey, your hand tuning was not good enough. Start over.*
2. Use the auto-correct buttons in the **C1A1** tab to correct the low order aberrations. It is usually safe to simply press **0th-2nd**⁷ with 100% strength. If this overshoots, use 75% or 50% strength.+ Repeat this until the entire line of measurements is white (or a very pale yellow). This should take no more than a few iterations.
3. The probe corrector software uses **Defocus** to adjust C1 when using the auto-correction buttons. If the defocus correction gets above, say, 10 nm, press **Eucentric Focus** and restore focus with the Piezo Z.
4. The A1 and A2 buttons have interactions with higher order aberrations, which become important later when we are tuning the high orders. This is discussed in detail in Section 3.6.3.

⁷ The WD control (beam tilt) is very sensitive to drift of the sample, so make sure the sample is very stable before correcting WD. If you switch back out of diffraction and the halo is no longer centered on the hotspot after correcting WD, this is normal and does not need to be fixed.

3.6.2. High Orders

On modern correctors, which measure the 2nd order aberrations in the anachronistically-named “C1A1” tab, it is not necessary to run anything other than the Enhanced tableau measurement, as by this stage the second order aberrations should be

corrected. On older correctors, A2 and B2 are fixed by running a Standard tableau first.

1. Go to the **Tableau** tab. Start an Enhanced tableau with 40 mrad outer tilt angle. When the tableau is complete, hit **Accept** and you will be brought to the correction tab.
 - Every blob in the tableau should have a green box around it after the measurement. If this is not the case, your second order aberrations are probably unacceptably large. Go back to C1A1 if this occurs.
 - Similarly, the C1A1 measurement for each tilt should be colored yellow at worst. If any are red, you probably messed up the hand tuning somehow. If any are grey, you almost definitely did not tune well enough. Nevertheless, if you made it this far and the software lets you accept the measurement, you can probably still continue on and correct using the autocorrect tools. (It's also possible that the higher order aberrations are just really high, and there's nothing you can do about that by hand!)
 - If a purple error message complaining about image shifts being too large appears in the text box at the bottom of the window, you will not be able to accept the tableau measurement. This is caused by the sample being at the wrong height. Go back to Section 3.4 and improve the sample height, set **Intensity List (FOCUS)** appropriately, and repeat all steps from that point.
2. In the correction tab, you will be presented with a table of the measured aberration coefficients, as well as the computed phase plate of the current alignment state. The calculated probe shape is shown in the bottom right. In this window, *aberrations shown in yellow indicate that the measured value is larger than the confidence window*. This means that you should *only attempt to correct aberrations that are shown in yellow*. Aberrations colored in white are measured with too low confidence to correct appropriately. There are several strategies to decide which aberration to correct:
 - Consult the table of achievable values in Section 2.3.1 (or a similar table of limiting values cus-

tomized to your liking) and correct any coefficients larger than the ideal (while of course only correcting the ones shown in yellow)

- The computed phase plate in the top right shows the current maximum angle with less than $\pi/2$ phase shift, and the aberration named in green is the one most substantially contributing to this limit. If the green aberration is colored yellow, correct that. (Note: make sure to choose “Exclude 1st & 2nd Order” in the display, there is no point in correcting low orders here).
 - The computed probe shape in the bottom right shows the radius containing half the probe intensity, and the aberration shown in blue is the one most contributing to this size. If the blue aberration is colored yellow, correct that
 - **Do not correct first or second order aberrations using the Enhanced tableau measurements. Only correct 3rd and 4th order.**
3. Apply one or two corrections from the tableau measurement. You can use 100% on the first few iterations, but as you improve things you should go down to 75% or 50% strength. The 3rd order correction buttons are well calibrated and can be used at high strength. The D4 and A4 buttons are usually okay, but should be approached more carefully. The B4 button is often not well-behaved.
 4.

If you are uncertain about applying a correction (in particular if you are correcting the 4th order aberrations), it is recommended to save the state of the corrector first so that you can recall it in case the correction makes the alignment worse. Click the yellow arrow with green circle icon near the top (it is captioned something like “save undo point”). If the corrections you apply are not good, click the other yellow arrow to restore these known good settings.
 5. After you have applied some corrections, repeat the cycle starting from Section 3.6.1. Perform a C1A1 and fully correct the 0th through 2nd order aberrations, as these are commonly induced as side effects of the higher order corrections. Then, run a new tableau and correct higher orders.
 6. To decide when to stop this cycle, you may consider the limit of the green circle: if it reads around 35 mrad (and

you intend to operate at 30 mrad), then you are sufficiently corrected. You may also use the calculated probe size as a stopping point (the value to stop at will be high-tension dependent, but the software reports the ideal probe radius for a given voltage, aperture, and probe current).

7. You may also decide to stop by checking the resolution by high magnification imaging. Zoom in to a very thin part of the tuning grid, and manually adjust the image using the **Condenser Stigmator** (note that you should not have touched this control at all before this step!). Acquire an image at around 3 Mx magnification with a sufficient (10 μ s or so) dwell time, and check the highest Fourier coefficient recorded, as well as the isotropy of information transfer.
8. If you reach a point where the software cannot measure any aberration coefficients large enough to limit the resolution, but you cannot actually achieve high resolution, this likely indicates the measurement noise is too high. You may increase the image acquisition time to get better signal. Also, check that you have sufficient probe current (CEOS recommends 100-200 pA, but we seem to still be successful with 50 pA). You may also increase the magnification now that the aberrations are improved, but you cannot go too high (450 kx or 600 kx is probably a reasonable limit).
9. Due to drift and interaction with the sample holder, you will have to adjust A1 and B2 once you remove the tuning grid and switch to your sample. You can do this by hand, with Sherpa, or by running a C1A1 on the platinum protection layer on a FIB lamella.

3.6.3. Control Impurity

As we've alluded to earlier in the manual, some aberrations can be produced by misalignments of the beam in multiple locations within the corrector. As a consequence, certain controls work in different ways depending on the magnitude of the aberration, with the two mechanisms having different side effects. Two such controls, whose side effects have been pointed out to me by Bin Jiang, are A1 and A2, which mix with S3 and D4, respectively:

The **A1_coarse** control shifts the beam in the hexapoles, while the **A1_fine** control uses QPx and QPy, a pair of quadrupole stigmators located after the second hexapole. When using the combined controls, the corrector will use **A1_coarse** as long as the magnitude is greater than its finest step, then for small changes it uses **A1_fine**. **S3** also uses QPx and QPy, and so there can be substantial crosstalk between these controls. At low voltage (60 kV) the smallest step of the **A1_coarse** control corresponds to around 20 nm of A1, and using the fine control to null this remaining A1 has side effects of about 600 nm of S3. There is not much to do about this coupling in tuning, but managing the QPx and QPy as you fight drift of A1 during a session is important to prevent growth of S3. After changing samples and after some time, you may want to reset the quadrupoles by zeroing the **A1_fine** control⁷, then using **A1_coarse** to fix the A1 as well as possible before stigmating with the fine control again.

The **A2_coarse** control uses the excitation of the main hexapoles, while **A2_fine** uses HPx and HPy, a pair of weak hexapoles after the final main hexapole. **D4** also uses HPx and HPy, and so these two controls are also coupled. In this case, it can be advantageous to adjust the correction procedure slightly to avoid dealing with too much crosstalk. Adjusting A2 by hand using the **A2_coarse** control until its magnitude is below about 100 nm before switching to the auto-correction tools can prevent bouncing between these two tools too many times. It's usually possible to reach 100 nm of A2 by eye, or you can use the manual **A2_coarse** control while watching the measurements from C1A1.

4. Zen and the Art of Probe Correction

This isn't a very good manual. The probe corrector is sufficiently complex that it takes experience and practice to master it. You need to converse with it, to poke it and prod it, listen to how it responds, and let it take you on a journey. In doing so you will sharpen your mental image of how it reacts, and what it takes to make it happy. A manual that rigidly prescribes every step in excruciating detail isn't a good manual either. A manual like that not only leaves out a lot of details (just as

⁷ The **Condenser Stigmator** in the microscope UI is the same as **A1_fine**, so you can zero it there. In the service mode GUI, you can use the **Reset A1_fine** button. The value shown in the Manual Correction tab is relative, so zeroing it there is not the same.

mine does) but also discourages exploration and stymies intuition. My manual is a condensation of many conversations I have had with the corrector, abridged and massaged and told by a biased narrator. I wouldn't write it any other way.

In Section 1 I've described a small fraction of the inner workings of this thing, in a way that I hope will help you to appreciate why I've been doing certain steps in a certain order. But in reality there are so many more dimensions of complexity that I can't yet even begin to understand, that I cannot truly convey everything that is going on. There are something like 40 different lenses, deflectors, stigmators, or whatever, inside the probe corrector alone (and perhaps another 20 in the rest of the condenser system). And this complexity turns out to be profoundly necessary: the basic sketch of the system was dreamt up in the 1940s [2]–[4], but it took half a century to work out all the places where you need to give the beam a little tweak, a subtle squeeze, a minute compression, to get this thing to *actually* deliver a sub-Ångström probe [5], [6].

With so many controls and so many ways to assess the state of the thing, there is no one right way to tune: there are practically infinitely many. There are also many dead ends, and I try to guide you away from those. There are so many dead ends, in fact, that without some sort of guide you are unlikely to ever reach your destination. But there is an undo button! You can let things get awkward and let the conversation go off the rails, and then when things feel hopeless you can just magically turn back the clock. You can start over from scratch over and over again, until you perfect your rhythm and you are practically *in love* with the probe corrector. If only the real world were so forgiving.

The best way to use this manual is to use it as little as possible. Read it over, go through the steps a few times with it by your side, and see if my style resonates. Experiment and explore, and if you get lost try your best to rescue things. You will learn far more by doing something *wrong* and taking the time to make it right than you will by memorizing this manual, or by following it blindly. But never forget you have that reset button—sometimes the conversation goes so awry you have to walk away to preserve your sanity. As soon as you are able, run through the entire procedure without looking at the manual.

Read it afterwards, and compare notes. Then, as you establish your own rapport with the machine, abandon the manual entirely.

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