Fast automated energy changes at GM/CA ID beamlines equipped with transfocator and focusing mirrors

Sergey Stepanov, David Kissick, Oleg Makarov, Mark Hilgart,

Michael Becker, Nagarajan Venugopalan, Shenglan Xu,

Janet L. Smith, and Robert F. Fischetti

APS TWG meeting, February 24, 2022

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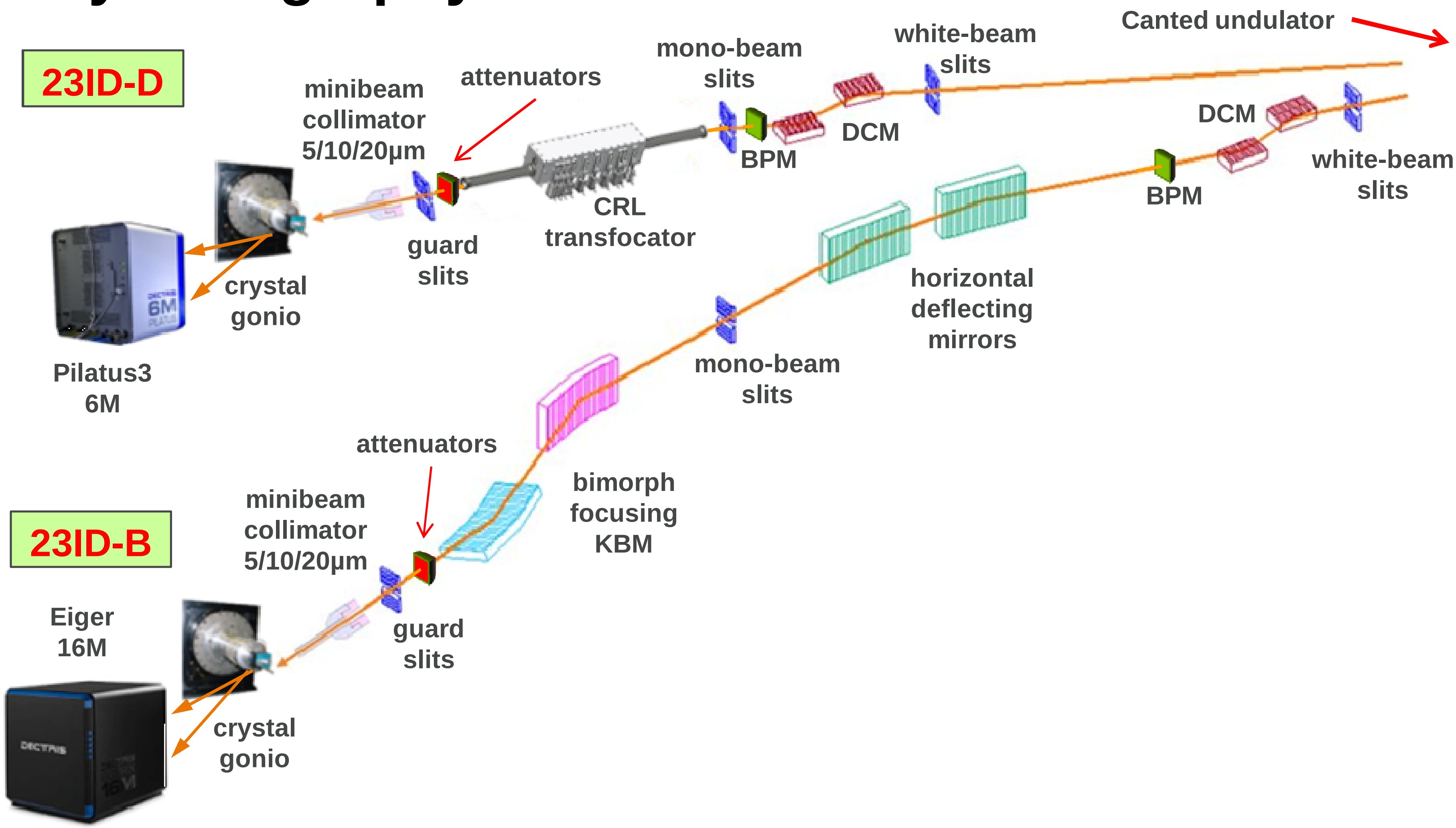
Rationales for automating energy changes

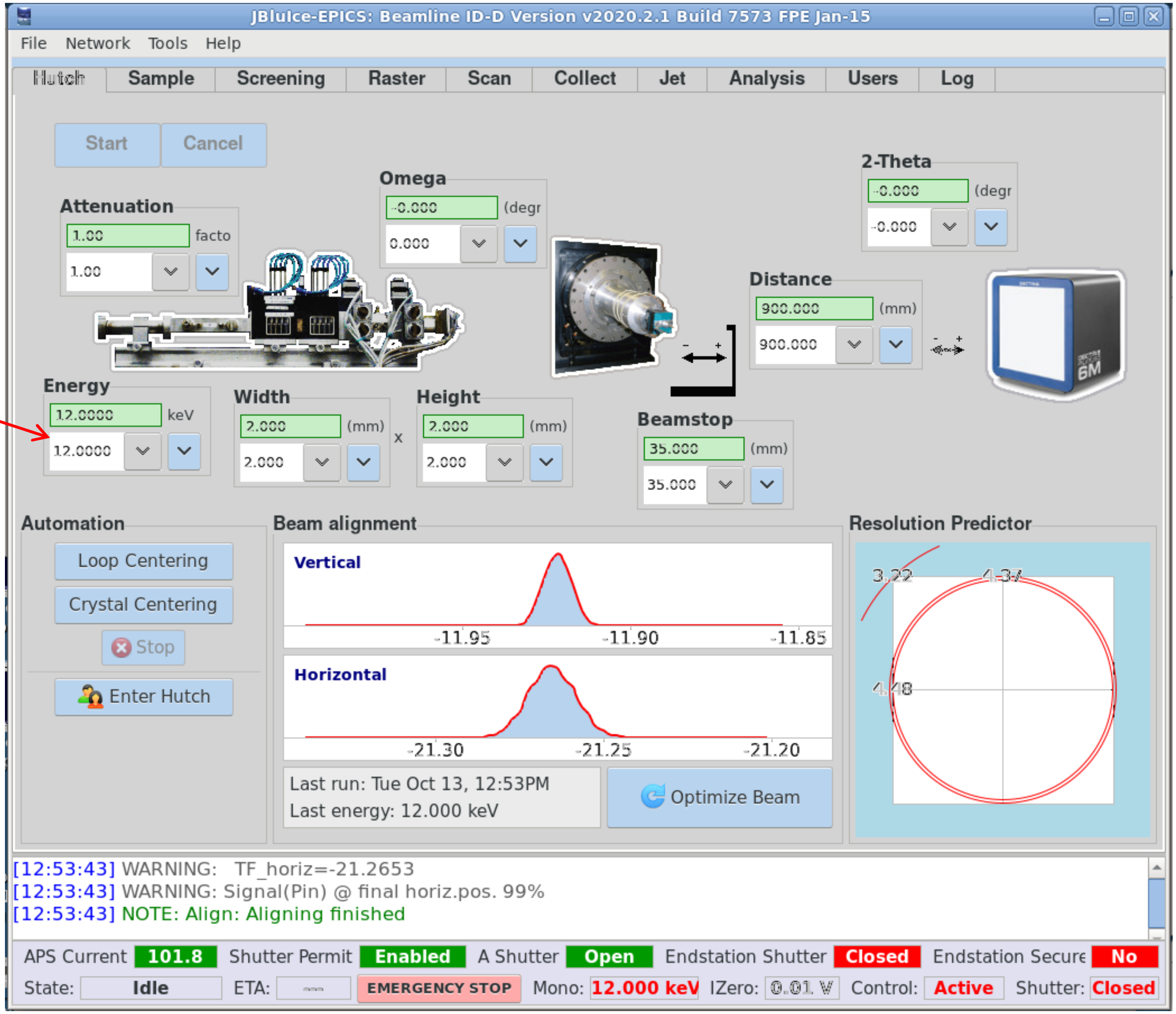
- At MX beamlines where typical beam time allocated for an experiment ranges between 6 and 24 hours and users often need to switch beamline energy to different absorption edges differing by several to a dozen KeV.
- In most cases, users and lately, due to the pandemic, even support staff, are remote. Obviously, for such short experiments, changing beamline energy should be as simple, smooth, and fast as possible.
- Because of pandemic, non-MX APS beamlines have also switched to remote operations. Therefore, we expect that automating energy changes currently presents a value for the broader synchrotron radiation community than just MX.

GM/CA 23ID beamlines layout: two canted undulator beamlines for macromolecular crystallography



Changing energy: users prospect

Dial new value



Changing energy: behind the scenes

1. Synchronously control the beamline monochromator and undulator to maintain the X-ray beam flux after the monochromator (keep intensity feedback happy).
2. Preserve beam attenuation by determining a new set of attenuator foils.
3. Change, as needed, mirror reflecting stripes, the undulator harmonic, and the Bragg reflection (111 <=> 333).
4. Preserve beam focal distance of compound refractive lens (CRL) focusing by changing the In/Out combination of lenses in the transfocator and shifting the transfocator Up/Down stream.
5. Optionally give system time for thermo stabilization.
6. Restore beam position at the sample by on-the-fly scanning of either the Kirkpatrick–Baez mirror angles or the transfocator up/down and inboard/outboard positions.
7. Protect the sample from radiation damage by automatically moving it out of the beam during the energy change and optimization.

1/7. Intensity feedback and synchronizing monochromator and undulator

When changing energy at ID beamlines a key point is to keep the ID and the mono roughly synchronized over energy during the change so that the beamline intensity feedback stays locked. If the lock is lost, searching for beam with the 2nd crystal pitch angle scanning may take long time.

Beamline intensity feedback is a software/hardware tool aimed at maintaining the second monochromator crystal parallel to the first crystal so that the monochromator passes a beam of maximum intensity. It continuously dithers the second crystal angle with a piezo actuator, checks for an increase or decrease in the beam flux after the monochromator, and then drives the angle in the direction of greater intensity.

Three algorithms for synchronizing ID and mono during the changes:

1. ID scan mode. The speed of ID is reduced so that both mono & ID accomplish the change in the same time. Problem: ID speed is constand over gap and mono speed over Bragg angle, but neither over energy. Therefore good for up to ~ 1keV changes.
2. ID steps mode. Mono moves to new energy continuously, but ID steps, every time ~100eV ahead of current mono energy. Works well with fast intensity feedback; little time overhead compared to method-1.
3. Multi-step mode. The change is split over ~250eV segments with little time between them for the intensity feedback to lock. Most stable, with ~6-8s overhead per 1keV of energy change.

2/7. Preservation of beam attenuation by determining a new set of attenuator foils

At GM/CA, the beam attenuation box contains 16 Ag and Al foils that can be inserted into or removed from the beam path to provide the requested attenuation. The box is located downstream of the focusing optics. When the X-ray energy changes, the efficiency of the foils also changes, and a new foil combination needs to be found in order to maintain the beam attenuation. This is recalculated in the loop carrying out the energy change in all three monochromator-ID synchronizing modes.

Without this recalculation, the attenuation could be greatly reduced when driving to a higher energy, and the sample would receive an unintended high dose if the energy is changed with the sample shutter being open.

3/7. Changing mirror reflecting stripes, the undulator harmonic, and the Bragg reflection

When moving to a higher energy, the angle of X-ray total external reflection from the beamline mirrors decreases, and then the mirrors may stop passing the beam. To prevent this problem, GM/CA mirrors have three stripes corresponding to different cutoff energies : bare Si, Rh-coated and Pt-coated. When moving to a higher energy, the mirrors are switched from Si to the higher-Z Rh, and then to the even higher-Z Pt. When going back to lower energy, the mirrors are switched back from Pt to Rh and Si to avoid passing higher X-ray harmonics from the undulator. At beamline 23ID-D the switching is required at 9.35 and 18.5 keV, respectively. At beamline 23ID-B, which additionally has two horizontal deflecting mirrors, the switching is required at 9.35 and 15 keV. Since the mirrors are downstream of the intensity feedback system, it is not required to synchronize the stripes changes with monochromator motion. Therefore, mirror stripes are changed before increasing energy and after decreasing.

Some energy changes require changing the undulator harmonic as the minimum or maximum ID gap is reached. At the GM/CA beamlines this occurs at 15 keV, 24 keV and 34 keV, which are the limits for the first, third and fifth harmonics, respectively.

At high energies (above 20 keV in the case of GM/CA beamlines) the monochromators can no longer use the 111 Bragg reflection because the second crystal translation reaches the travel limit and the monochromator needs to be switched to the 333 Bragg reflection.

At the threshold energies corresponding to the ID harmonic or Bragg reflection switching, the energy change and intensity feedback are **paused** until the switching finishes.

4/7. Preserving beam focal distance with CRL transfocator

Beamline 23ID-D was recently upgraded: a compound refractive lens (CRL) transfocator with parabolic lenses instead of a KBM system is used to provide a 2D micro-focusing capability.

When a beamline includes a CRL transfocator, which is a dispersive focusing device, it needs to be reconfigured to place a different CRL combination in the beam in order to preserve the focus and the remaining difference needs to be accommodated by shifting the transfocator up or downstream.

GM/CA CRL Transfocator: 19 groups (165 lenses) total; 14 groups (134 lenses) used below 20 keV. Lens radius: 500, 200, and 50µm. Device length: 498 mm (375 mm without 50 µm lenses). Distance from source 70.5 m; distance from sample location (focusing point) 1538.8 mm.

4/7. Preserving beam focal distance with CRL transfocator (continued)

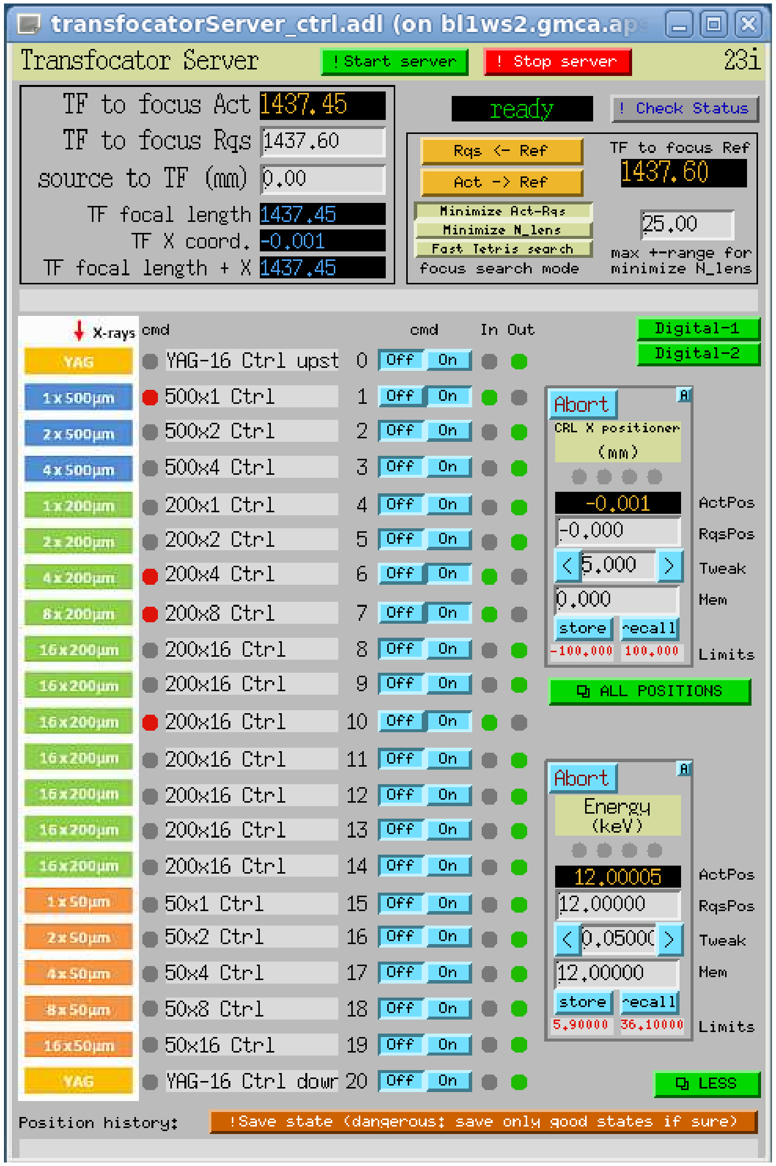
We have developed a Transfocator Server (TS) using the Bruls recursive equations (Optik, **126**, 659–662, 2015) to calculate the focal distance:

$$P_n^{overall} = P_{n-1}^{overall} + P_n\left(1 - \sum_{i=1}^{n-1} P_i^{overall} D_{i(i+1)}\right)$$

where $P_i = 1/f_i$ is the optical power of each lens block, $D_{i(i+1)}$ is the distance between the lens blocks. The overall focal distance $f_n^{overall} = 1/P_n^{overall}$ of the transfocator is counted from the rear (downstream) principal optical plane P_R of the current lens stack:

$$P_R - L_n = f_n^{overall}\sum_{i=1}^{n-1} P_i^{overall} D_{i(i+1)}$$

L_n is the position of the last (most downstream) lens block inserted into the beam.



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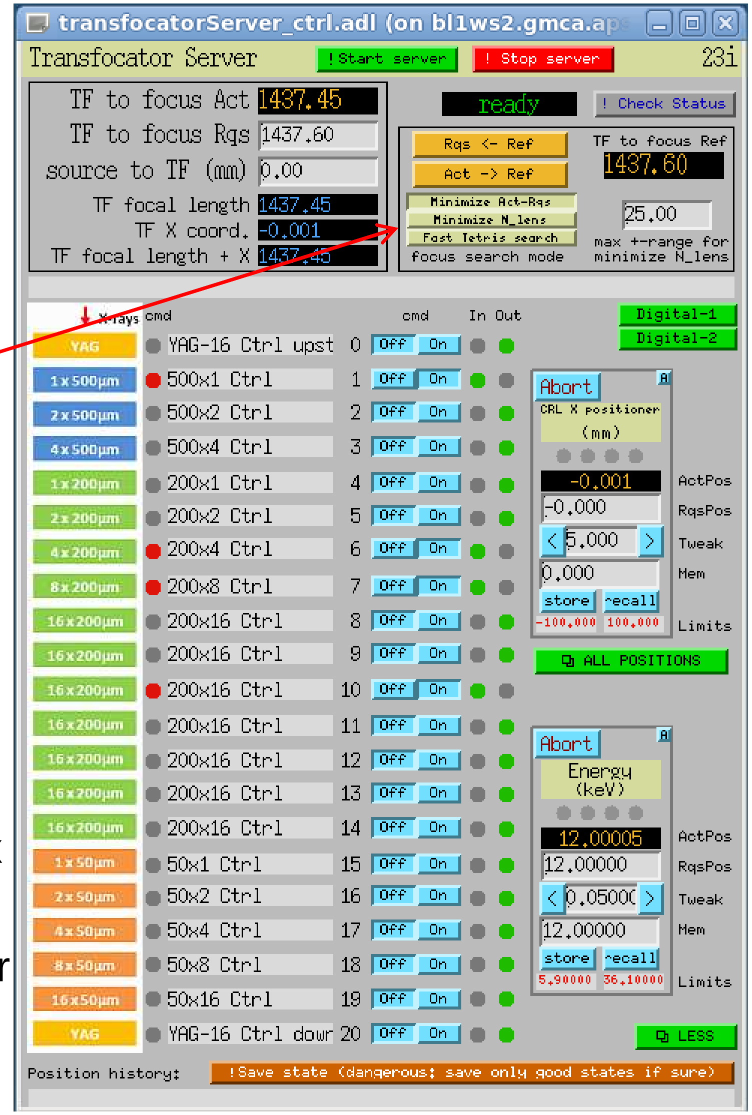
4/7. Preserving beam focal distance with CRL transfocator (continued)

When new energy is requested, Transfocator Server is requested to find a combination of lens In/Out corresponding to the best match with the current focal distance. The remaining difference is accommodated by shifting the box.

Three search modes have been implemented (in all cases the Bruls equations are used for calculating the focal distances):

1. Minimize Act-Rqs: check all 2^{19} or 2^{14} lens combinations, sort them by difference from the requested focal distance and choose the smallest.
2. Minimize N_{Lens}: similar to method-1, but choose a combination with the smallest number of lenses in the beam within specified allowance (e.g. 25mm max difference).
3. Fast aka-tetris search: sort lens blocks by their power and start filling requested power with the most "powerful" blocks.



Methods 1 & 2 take 1s with 2^{14} and 30s with 2^{19} combinations. Method 3 is instant. Transfocator is reconfigured after the energy change.

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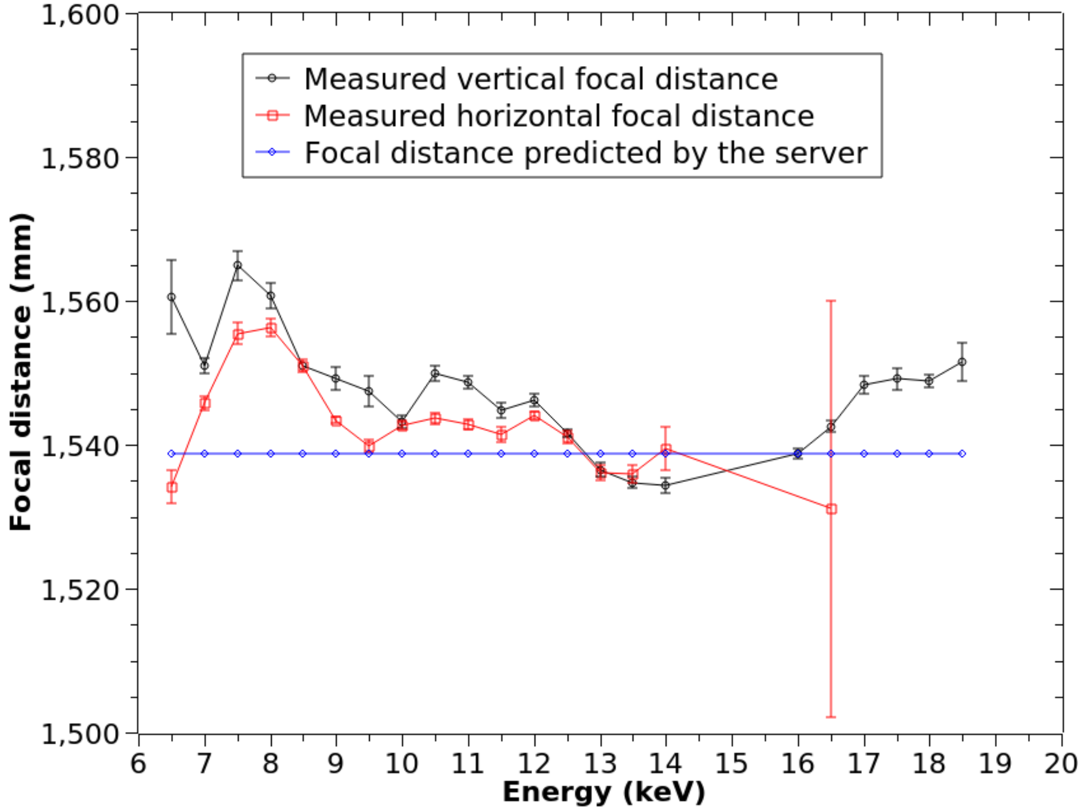
4/7. Preserving beam focal distance with CRL transfocator (continued)



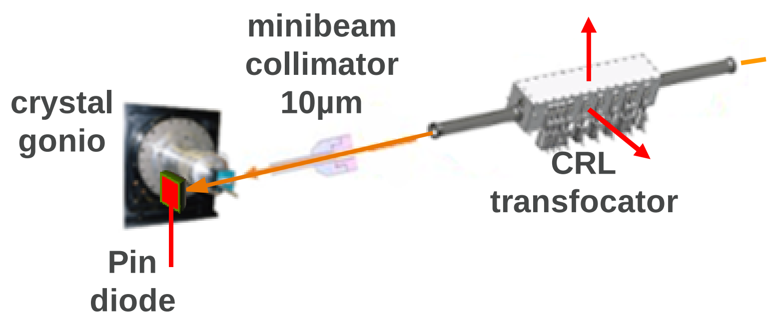
Predicted versus measured focal distances in the energy range from 6.5 to 18.5 keV. The horizontal measurements above 16.5 keV were too noisy and the error bars exceeded the mean deviations; therefore they are excluded. The magnitude of differences (< 25 mm) is expanded by the choice of Y-scale. Compared with the 1538.8 mm focal distance, which is the transfocator setpoint, they are minor (less than 1.69%).

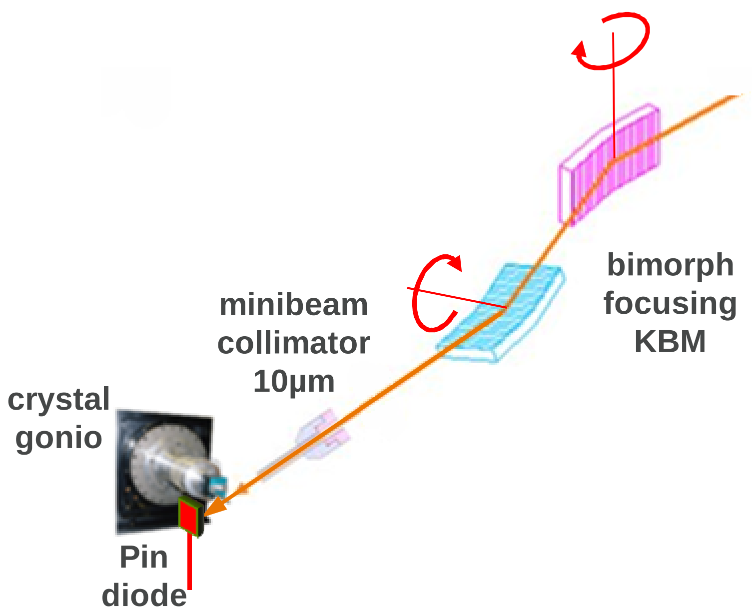
5/7. Optional thermo stabilization delay

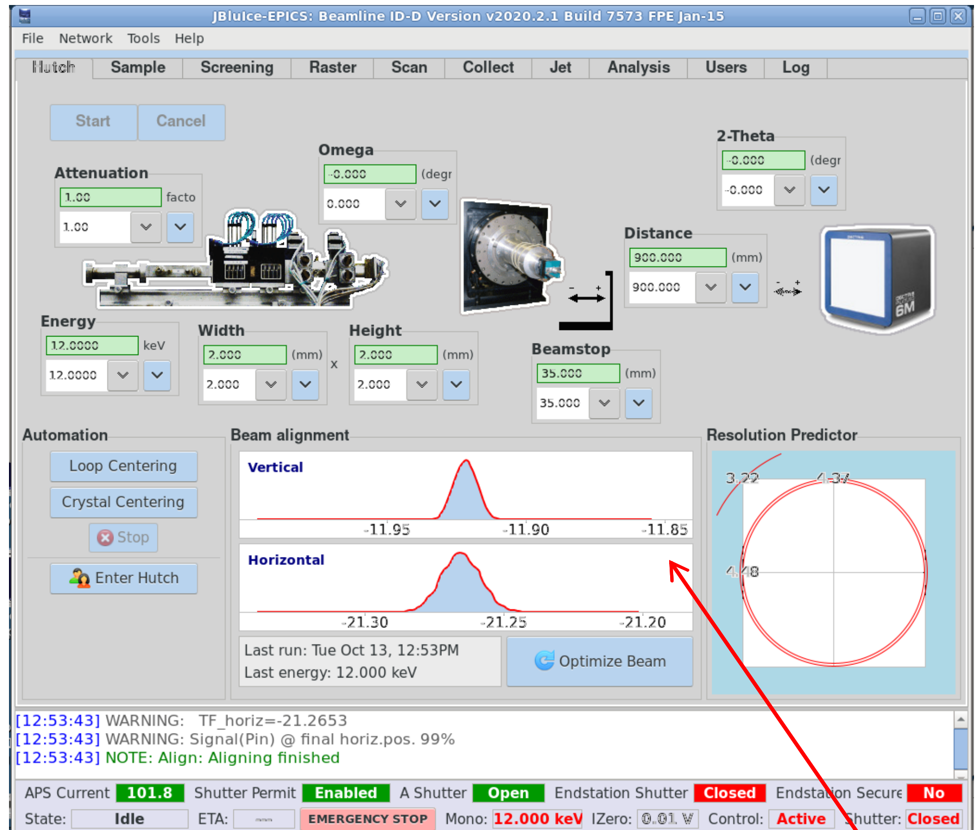
After the energy change is complete and before re-centering the beam at the sample software includes option to wait for the monochromator temperature stabilization after changed thermo load. The times are set empirically and calculated proportionally the energy difference from no wait for the changes under 1 keV to up to 2 minutes for the changes by 5 keV and more.

6/7. Restoring beam position at the sample

To re-center the beam after energy changes, software brings small 10µm pinhole collimator and a pin diode and carries out vertical and horizontal on-the-fly scans either with the CRL box positions (servo motors) or the KBM angles (DAC on the mirrors piezos).







Centering scans results

Centering is not initiated for small changes $|\Delta\theta_B| < 1°$

7/7. Sample protection

The sample is protected from radiation damage by automatically moving it out of the beam (shifting be several millimeters) during the energy change and optimization.

After the steps 1 to 6 are completed, the sample is returned.

A Hall sensor on the goniometer is used for detecting if a sample is present.

All steps in action: retuning from 12keV to 35keV

1. If sample is present on the goniometer, move it out of the beam
2. **12 keV** — If KBM present, start shifting them laterally from Si to Pt stripes
3. Synchronously tune monochromator and undulator to 15 keV
4. **15 keV** — Retune undulator from the 1st to the 3rd harmonic
5. Synchronously tune monochromator and undulator to 20 keV
6. **20 keV** — Retune monochromator from 111 to 333 Bragg reflection
7. Synchronously tune monochromator and undulator to 24 keV
8. **24 keV** — Retune undulator from the 3rd to the 5th harmonic
9. Synchronously tune monochromator and the ID to 34 keV
10. **34 keV** — Retune undulator from the 5th to the 7th harmonic
11. Synchronously tune monochromator and undularor to 35 keV
12. **35 keV** — If KBM present, verify that their shifts to Pt stripes have finished
13. If TF present, reconfigure the CRLs to initial focal length of 12 keV
14. Wait up to 2 min for monochromator thermo stabilization
15. Bring in Pin diode and 10μm pinhole and center the beam vertically and horizontally with scanning either KBM piezo or TF lateral pos.
16. If sample is present on the goniometer, return it into the beam

The entire process of reconfiguring the beamline from 12 to 35 keV including 2D alignment takes under 12 minutes. A large portion of this time is consumed by changing the ID harmonics and especially the Bragg reflection.

Smaller energy changes consume shorter time:

- retuning from 7 to 12 keV takes 4 min,
- from 12 to 16 keV which involves one ID harmonic change at 15 keV takes 6 min,
- from 12 to 13 keV consumes only 25s.

Conclusions and outlook

- Full reliable automation for changing beamline energy in wide range by users without staff help is feasible and works well: it is routinely used at GM/CA on daily basis
- Using CRL transfocators at beamlines with frequent energy changes and energy scanning is possible and can be made as easy as with KBM
- All software reported here is an open source distributed as a part of JBluIce-EPICS package (https://www.gmca.aps.anl.gov/jbluice-epics/). These are standalone scripts that can work without the JBluIce GUI. Therefore, adapting them should be relatively easy and mostly involve hardware interactions while re-using the algorithms
- More details can be found in the JSR paper which is coming in March, but already available at: https://doi.org/10.1107/S1600577522001084
- The GM/CA beamline 23ID-D is currently in the process of installing new bent focusing KBM to be used in combination with the CRL transfocator. The automations for the combined KBM + CRL system are going to be the next challenge, but based on our experience seem doable