PUSHING THE SPEED LIMIT OF HARDWARE-TRIGGERED SCANS

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1. MACROMOLECULAR CRYSTALLOGRAPHY (MX) AT DIAMOND LIGHT SOURCE

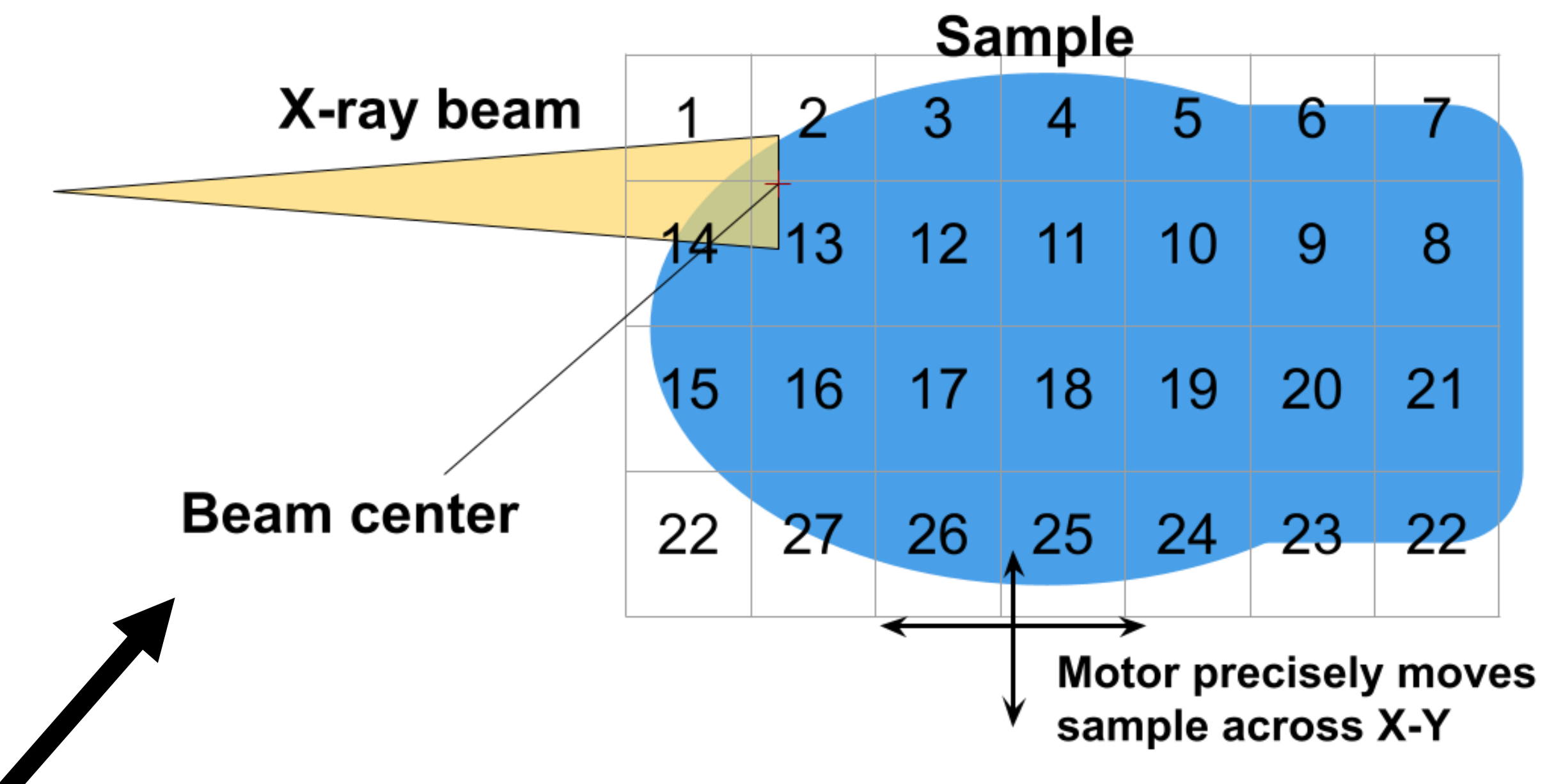
MX experiments aim to uncover the structure and behaviour of proteins, viruses, DNA, and other macromolecules. MX plays a crucial role in drug discovery, understanding of molecular mechanisms, and the advancing of medical research.

Diamond Light Source (DLS) have beamlines capable of doing these experiments without any interaction needed from the user - UDC (unattended data collection).

DLS are building an ultra-high throughput MX beamline which aims to collect from 5000 samples per day. To reach this target, every stage in the UDC process needs to be heavily optimised for speed, without compromising data quality.

Basic UDC loop
1. Robot loads pin containing sample into beam position
2. Optical camera used with centring algorithm to align pin tip
3. Grid scan: Sample scanned under x-ray in a raster trajectory to find which point of crystal diffract most strongly. **This is the part we are trying to speed up**
4. Data collection: Sample moved to best position and scanned under x-ray through a 360-degree rotation

2. X-RAY GRID SCAN FOR CRYSTAL CENTRING

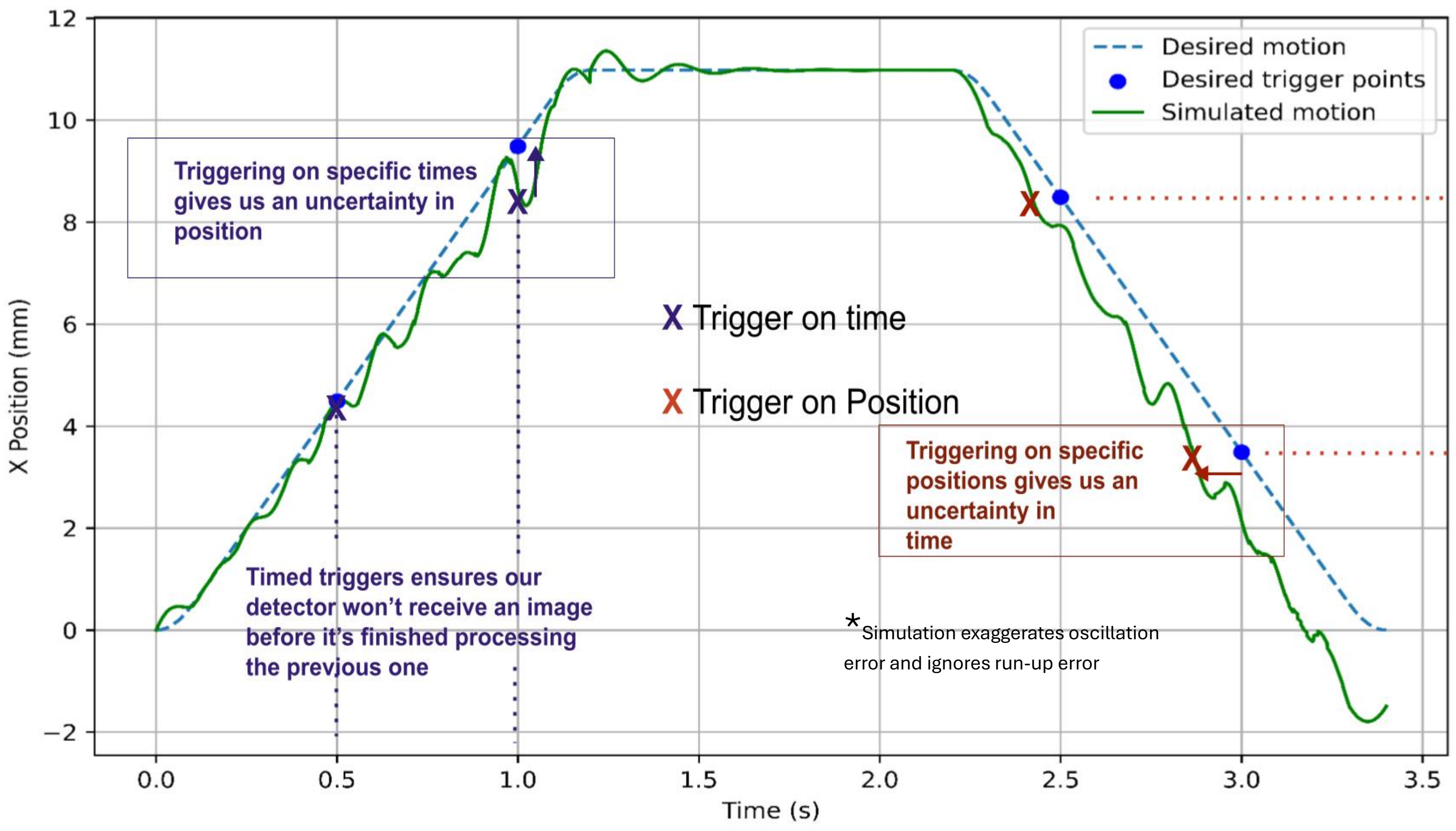


Using Bluesky, a virtual-grid is drawn across the pin, and a motion controller reads these grid parameters to calculate the path of the motor.

The pin is moved such that each grid box is scanned in ascending order.

3. WHAT IS LIMITING SCAN SPEED?

To get the fastest possible scan, we need to use the smallest allowed detector exposure time and the maximum possible motor speed. For the Eiger and Smargon, this is 0.2ms and 10mm/s respectively. Accurate scanning at this speed isn't easy.



We need to prevent sending detector triggers too frequently for images to process, but accumulative systematic error means scanning using only time-based triggers is too inaccurate.

Solution: At the beginning of each row, use one position-based trigger, followed by periodic time-triggers. By restarting our clock on the position trigger, we reset any accumulated error.

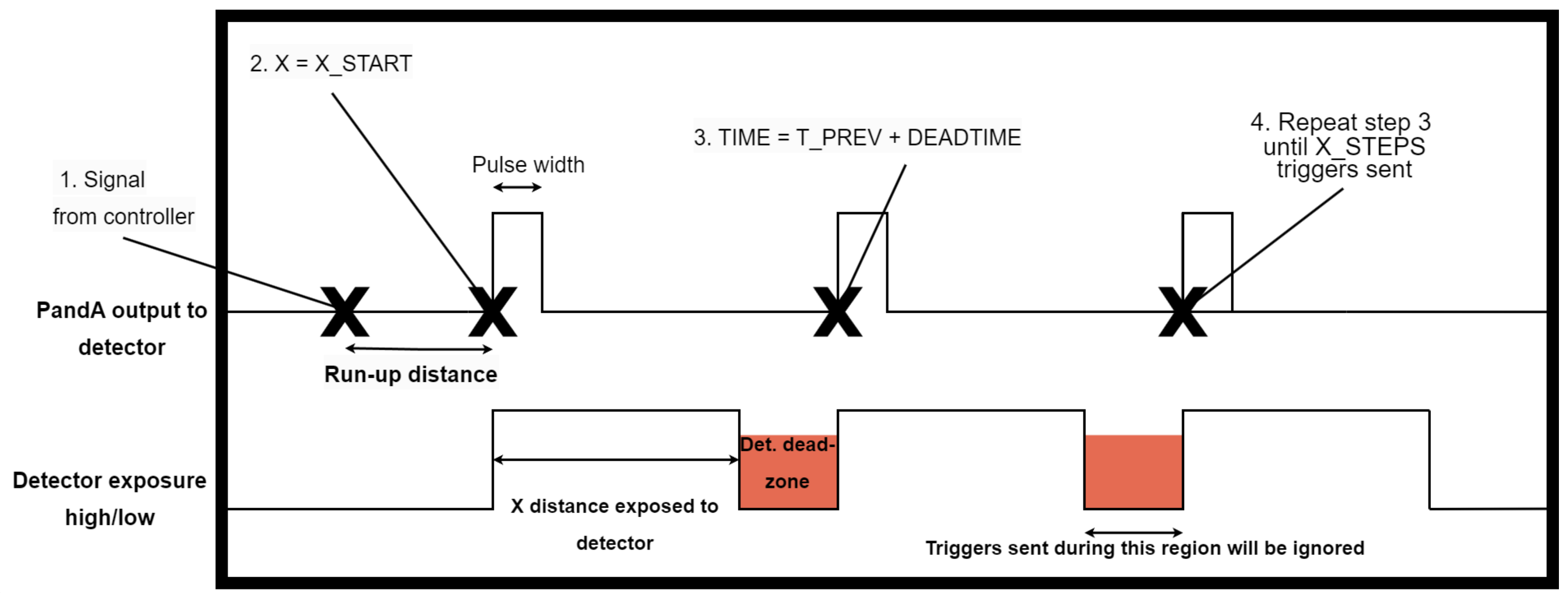
To do this, we need hardware which allows us to send signals based off a combination of position and time all in one configuration.

4. SOLUTION: TRIGGERING DETECTOR USING THE PANDA

The Position and Acquisition (PandA) box is a highly configurable pulse generator and data capture unit. A series of step-by-step conditions can be programmed into the PandA's Sequencer to specify detector triggering. The PandA can send pulses based off encoder signals from motors, as well as from an internal clock.

The table shows sequencer instructions for one row of the grid:

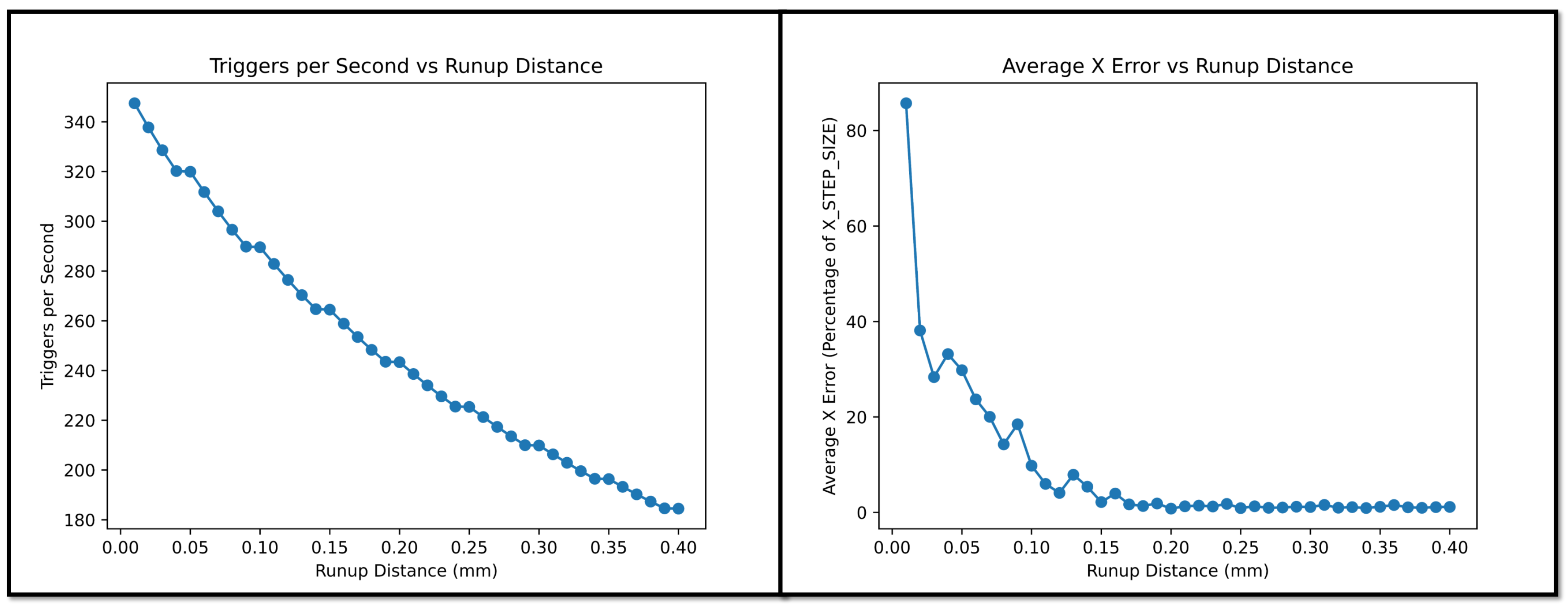
CONDITION	OUTPUT TO DETECTOR	TIME1	ACTION AFTER TIME1	ROW REPEATS
1. SIGNAL FROM CONTROLLER	0	0	NONE	0
2. POSITION: X = X_START	1	EXPOSURE TIME	OUTPUT = 0	0
3. TIME: T = T_PREV+DEADTIME	1	EXPOSURE TIME	OUTPUT = 0	X_STEPS



RUN-UP DISTANCE

Motors need space to accelerate and stabilise to their requested velocity and so a run-up is required at the beginning and end of each scan. However, this run-up distance has a negative impact on the overall speed of the scan and so a balance needs to be found between speed and accuracy.

Using the PandA's data capture feature, we can confidently choose a run-up distance which gives an acceptable accuracy during scans.

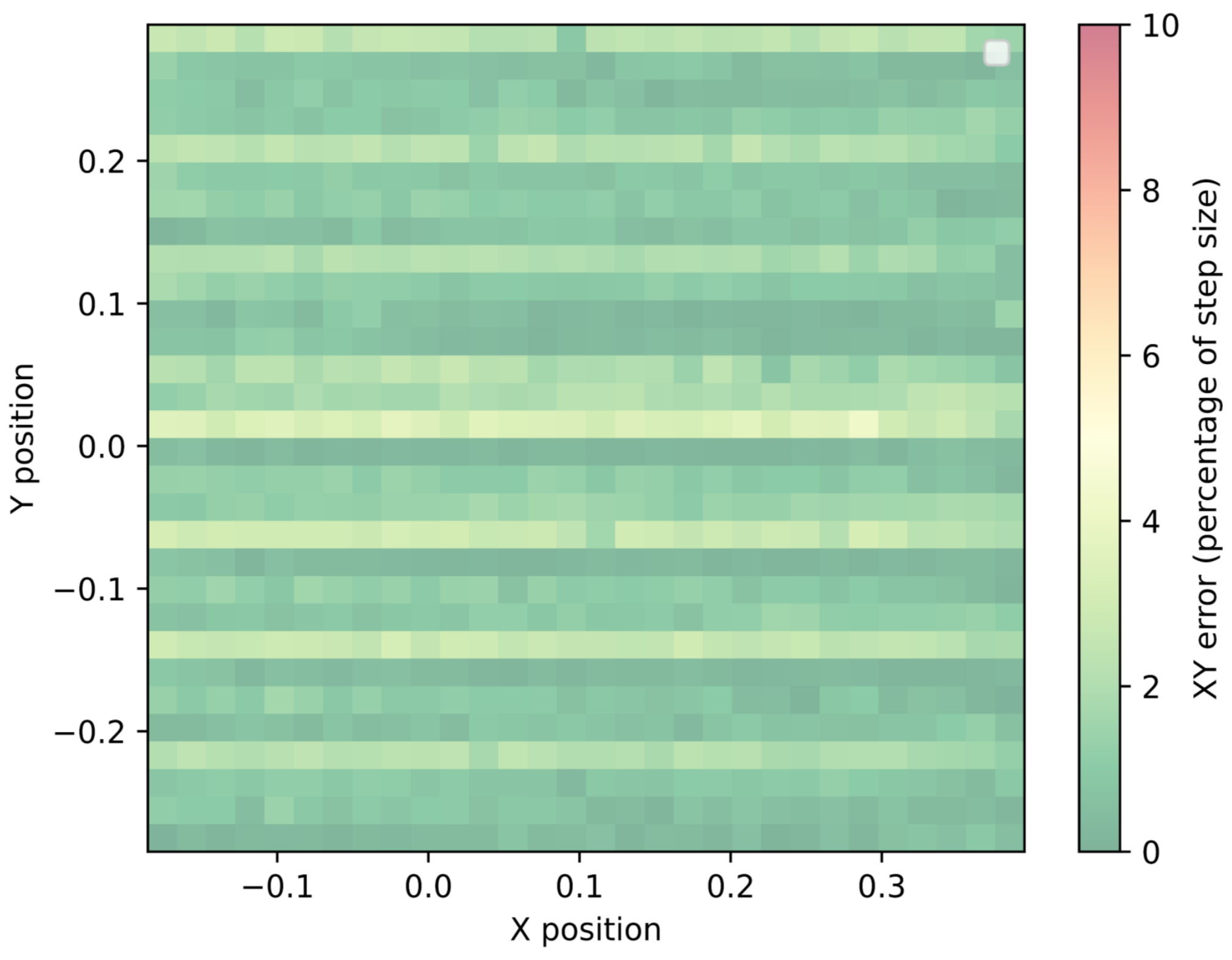


This data was gathered with a 30x30 grid. A larger grid will amplify any error coming from insufficient run-up distance.

The PandA data is captured immediately – corrections from small errors in position could be done within the UDC loop.

5. RESULTS

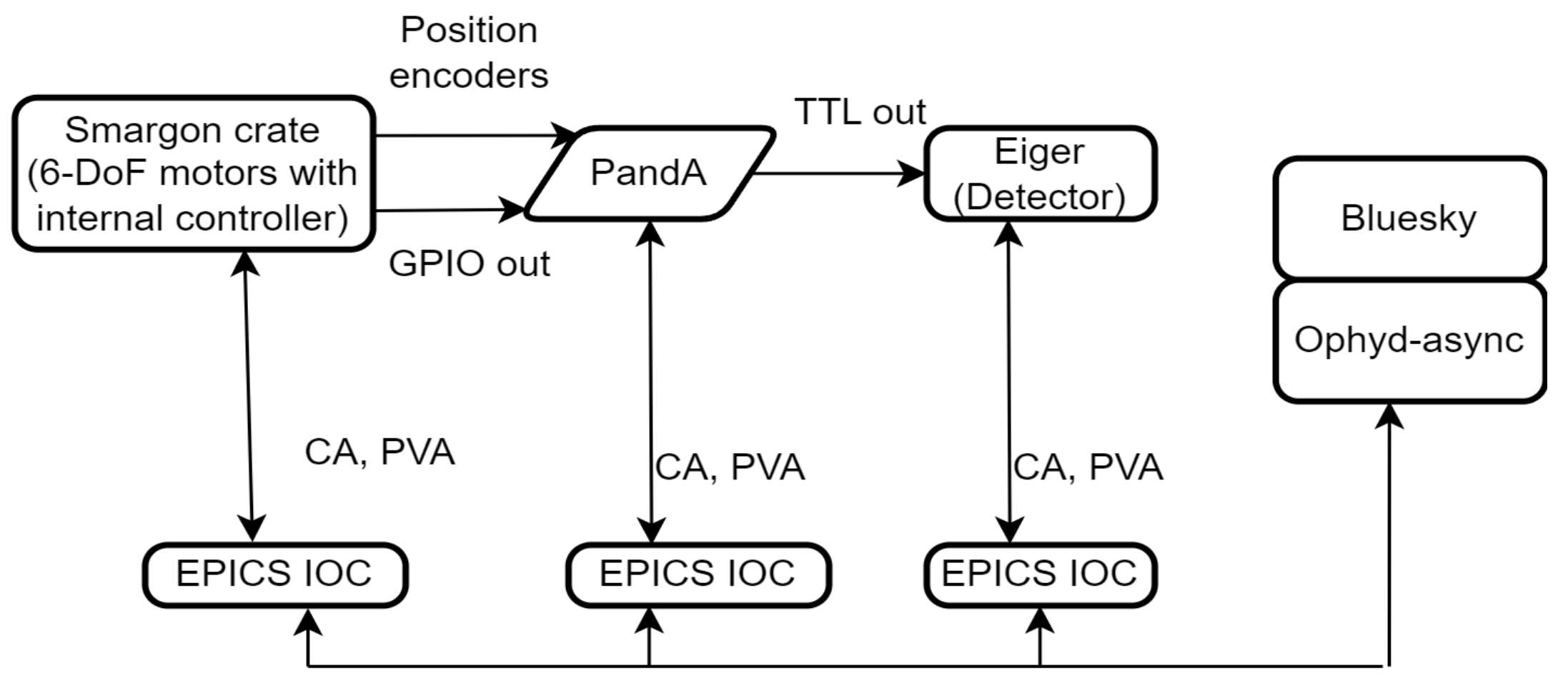
30x30 Grid Scan



Small error seen on some rows can be reduced using longer run-up distances.

- Extremely accurate scans using limits of the detector and motor
- Average X error: 1.6% of grid steps (using 20μm steps)
- Double speed compared to DLS's old grid scans
- Two grids of 900 points now complete in ~7s, including a rotation halfway through

BEAMLINE COMPONENTS



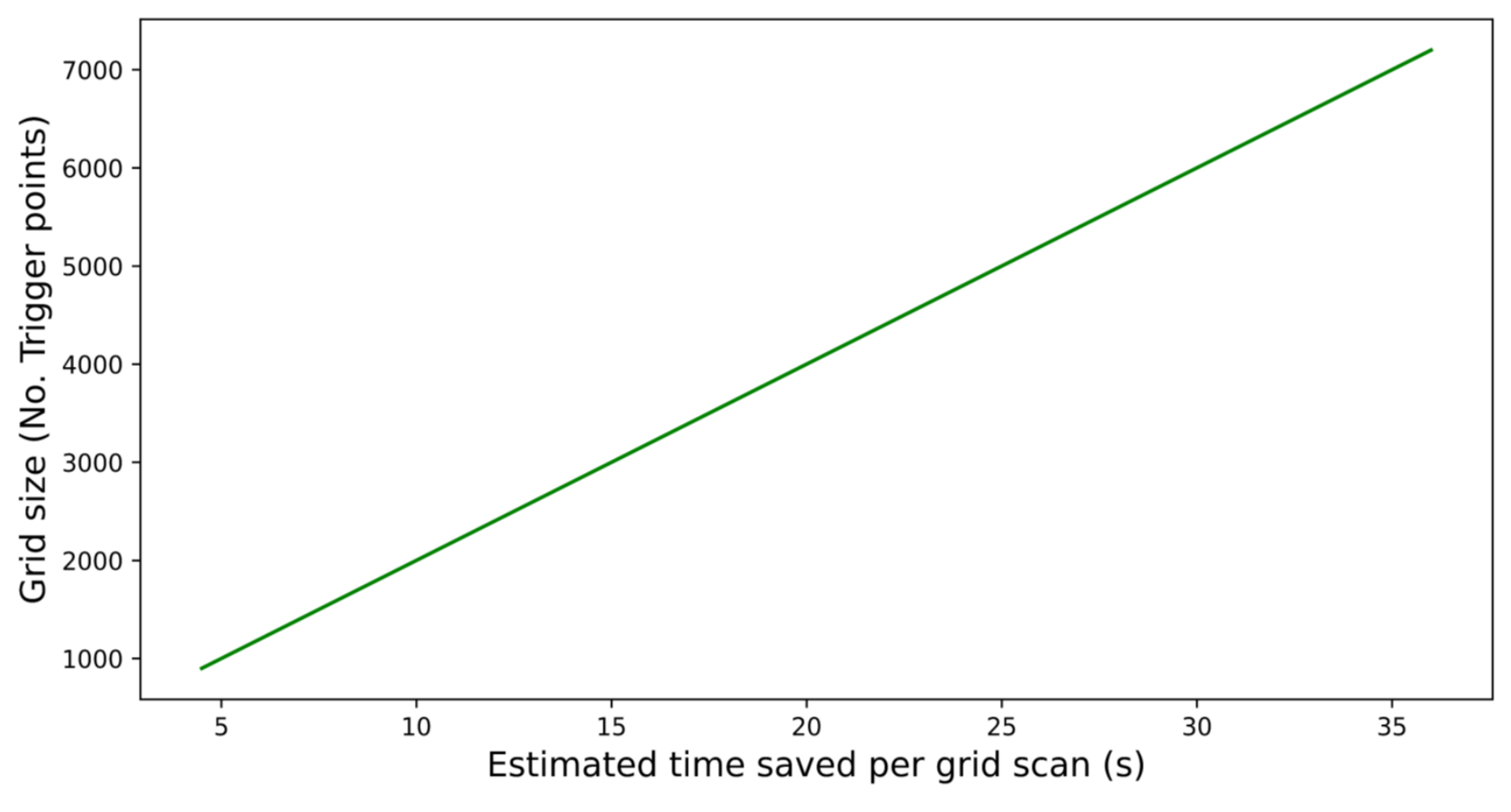
Bluesky is used to orchestrate experiments through a hardware abstraction layer, Ophyd-Async.

DLS uses EPICS for almost all hardware in beamlines.

Devices can be controlled and monitored through channel and process variable access (CA, PVA).

THE FUTURE : MULTIPLE SAMPLES PER PIN

By using a pin with 6 samples, throughput can be drastically increased. With 6x as many trigger points on the grid, optimising the grid scan becomes even more important.



- A data collection on DLS's I03 beamline currently takes 75s per sample
- Grid scan improvements have potential to massively increase samples per day

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For more information, please visit www.diamond.ac.uk or contact Oliver.Silvester@diamond.ac.uk