The Atlas X-Ray Diffractometer

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The background

The Atlas on-line X-Ray Diffractometer project (X-Rad, for short) was born at a time in the early 1960's when it was becoming clear computers and automation could have a massive impact on the speed and reliability of repetitive scientific processes requiring the collection of large amounts of data. The use of X-ray diffractometers to examine the internal structure of crystals at a molecular level is one such application. The principles were established by W L Bragg and his father in 1912 and have been widely exploited since. In particular, X-ray diffraction techniques have been fundamental in the determination of the 3-D structures of complex organic molecules, well known examples being penicillin and insulin. Both these structures were solved by the distinguished scientist Dorothy Hodgkin, awarded the Nobel Prize in 1964 for her work using X-ray crystallography, who visited the Manchester project in its later stage to see the work being done.

The size and cost of early computers made it unrealistic to dedicate a whole machine to a single scientific instrument. The notion of time sharing, as exemplified by Atlas, opened up the opportunity to control data collection just using a fraction of Atlas's capability and made the concept much more attractive. An important follow-on question was just how the work balance should best be shared between Atlas and the data collection system. But first, some background on the X-Rad system and the people involved.

Figure 1 shows the four-circle diffractometer, also called a goniometer, mounted on its cabinet containing the power supply and controls for the X-ray source. Alongside is a standard Atlas cabinet containing the digital and analogue electronics linking the diffractometer to Atlas. The diffractometer, a Y290, was designed by V W Arndt, then at the Royal Society, and made by the long-established, but sadly now defunct, precision instrument manufacturer Hilger and Watts in north London. An initial attempt to automate the Y290 had proved unreliable and the University of Manchester was given the opportunity to exploit the potential of Atlas in a novel way to achieve real-time data collection.

The equipment in Figure 1 was surrounded by a glazed cubicle, the whole being located about eight yards from the Atlas computer in a separate room previously occupied by a Mercury computer. Owen Mills from the University's Chemistry Department was the client, a specialist in X-ray crystallography and a major computer user. Dai Edwards took the lead responsibility for the Electrical Engineering Department. The other members of the team were Keith Bowden, who initially was also involved in the Atlas fixed-store design and implementation, and myself. I graduated in EE in 1961 and joined the group as an MSc student under Keith's supervision. My particular responsibilities lay with the position control systems for the diffractometer but, being the junior member, was also involved in the complete design and implementation process. A very satisfying experience.

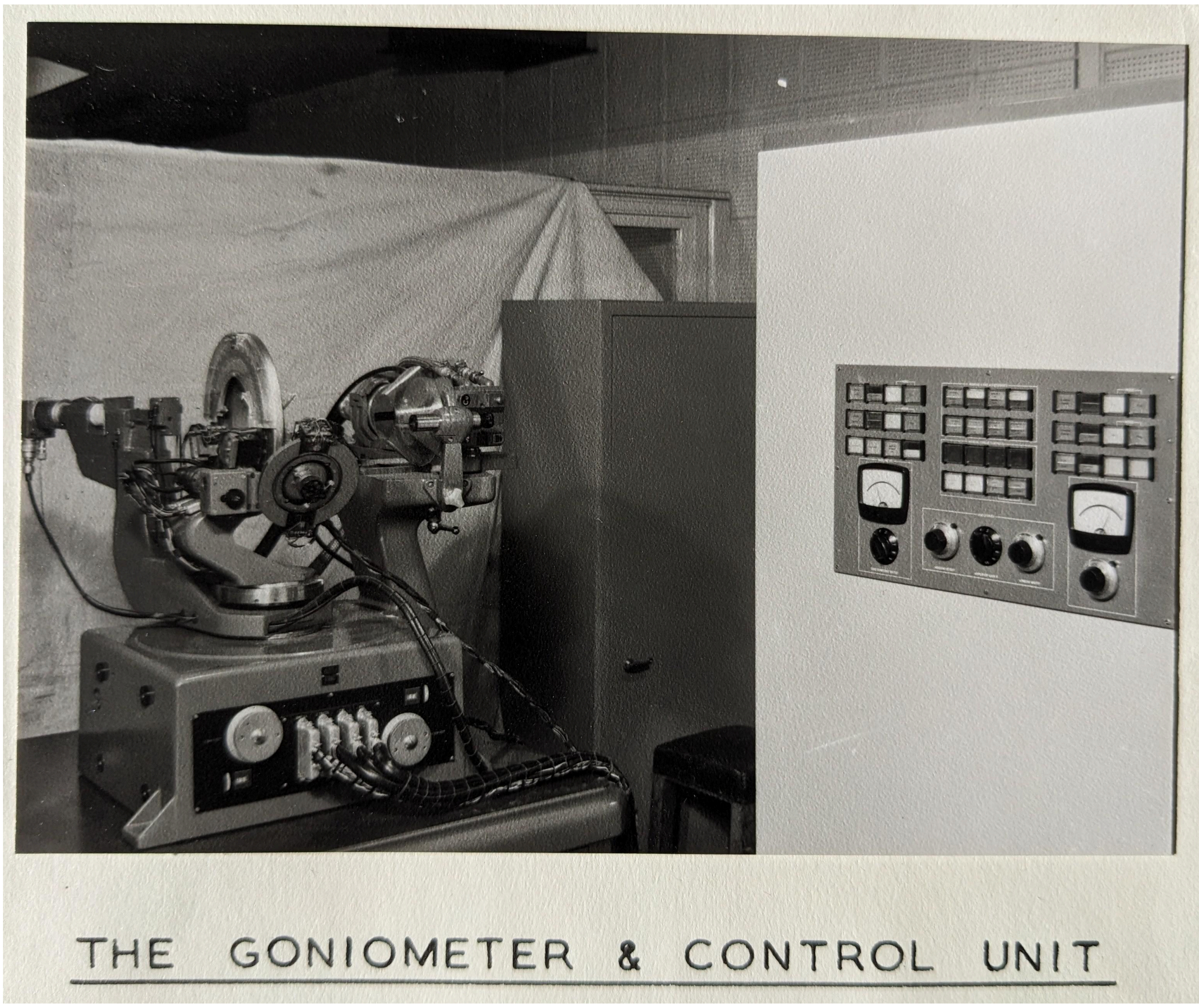

Figure 1. The four-circle diffractometer at the heart of the X-Rad system. To the right is shown the cabinet containing the electronics that linked the X-Rad system to the Manchester Atlas computer.

The system

The crystal whose structure is to be studied is mounted on a thin support so that it lies at the very centre of the diffractometer. Three separate circular components are visible in Figure 2, the *phi*, *kai* and *omega* circles. These can each rotate independently and be set to any position with an accuracy of 0.01degrees. So, it is possible to choose any angular position for the crystal in 3-dimensions to a high degree of accuracy. The fourth circle, *twotheta*, carries the X-ray detector. The detector can only rotate in one plane so, for each measurement position, the crystal must be set so the diffracted beam of interest lies in the detector plane. The diffracted beam has a natural spread and its intensity is measured by scanning the detector across the beam for a set time and counting the quanta received. The repetitive operating sequence of the diffractometer is to set a new crystal and detector position, generally involving movement of all four circles, followed by a scan of the beam using just two circles whilst measuring intensity. A data gathering session might involve several thousand measurements and take many hours. Overnight and weekend running was the norm. The results of a run were accumulated in a file (held on magnetic tape) on Atlas. At the conclusion of a run, an analysis program produced the desired information on the structure of the molecule under test.

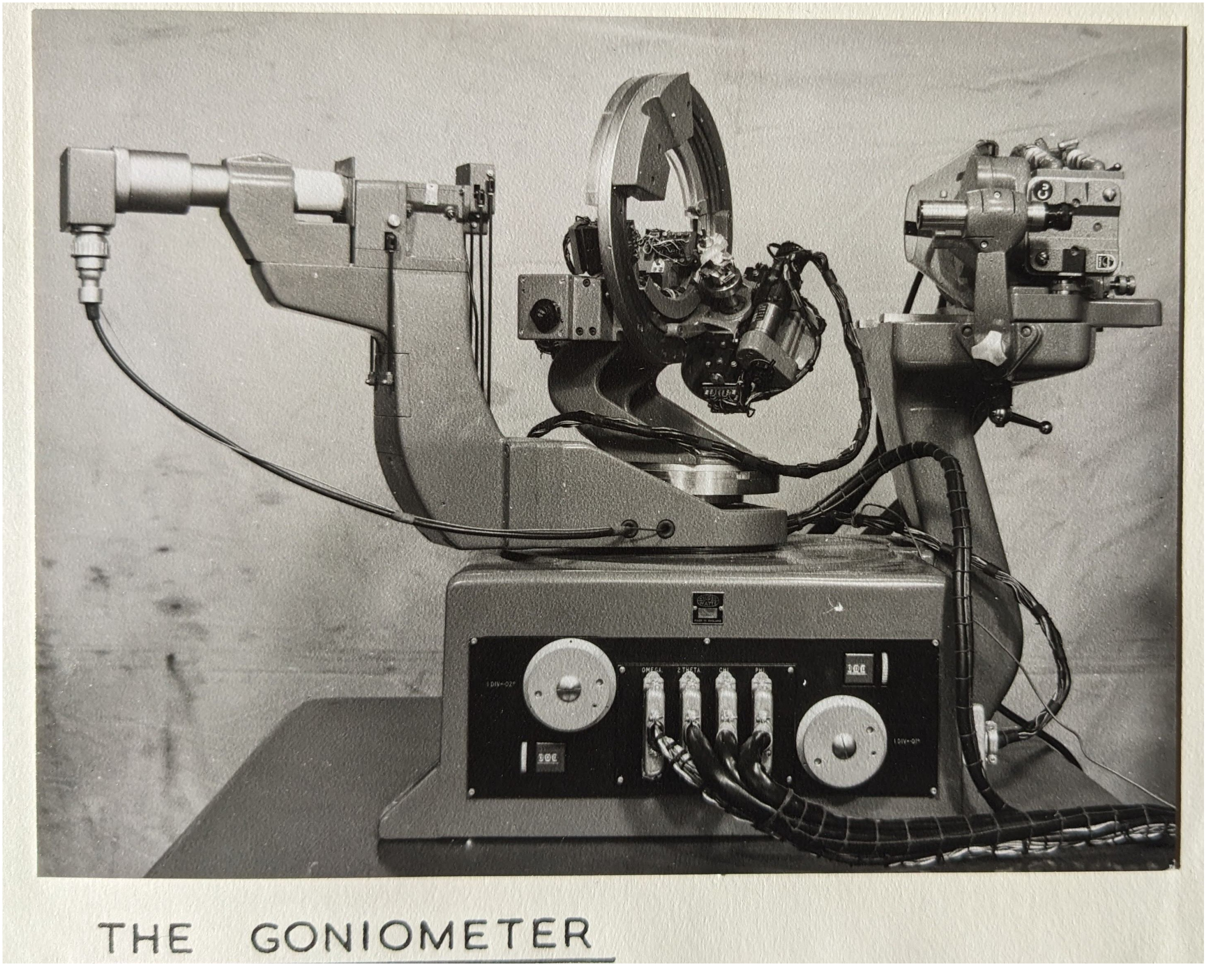

Figure 2. Close-up of the type Y290 diffractometer or goniometer at Manchester.

The motors for each of the four circles were state of the art DC permanent magnet motors with DC tachometers attached. This was before the days of digitally commutated motors. Conventional transistor power amplifiers drove the motors and speed was controlled by an analogue velodyne system. Angular movement was measured by optical Moire fringe systems of the type then being adopted for numerically controlled machine tools. Because the Moire fringe system provided relative rather than absolute positioning, a separate set of photocells scanned separate tracks with clear and opaque sections to set the working range of each circle. This allowed the diffractometer to find fixed reference positions from which all further movements were made counting fractions of the Moire fringes. Limit switches protected the diffractometer from malfunctions and positioning errors.

A party trick for visitors was to allow them to force a diffractometer circle away from its desired position using the manual setting wheels and then watch and feel the digital servo firmly but gently drive it back to exactly the right position.

The whole control system, including both analogue and digital sections, was mounted in a standard Atlas rack with Atlas circuit boards for the digital logic. Because both positioning and beam measurement just required simple arithmetic counting, the digital system was based around a set of registers and a half adder/subtractor. For diffracted beam measurement, 20 bit register capacity was chosen to give adequate statistical accuracy. Signed differences for positioning each circle within a 360degree range with 0.01degree accuracy requires 17 bits but 18 bit registers were chosen for engineering convenience. So, the register and half adder/subtractor data loop was set at 20 bits.

There is an interesting twist to the design that reflects the relatively high cost of digital circuits at that time. The total functional register capacity is just 72 bits for positioning the four circles and 40 bits for receiving the counts from two detectors (the Manchester chemists chose to use just one but the system was designed for the more general case with two). A mere 104 bits in total. However, it was thought worthwhile to share some registers between functions because not all are in use at one time. The digital position control loops for each of the circles could be kept live even when not moving to new positions by short, 6 bit, 'clamping' registers. The actual gain was minimal but from my memory of the design decisions it was thought worth the slight extra complication to demonstrate the principle.

Communication between the diffractometer system and Atlas was via the standard Atlas V-store system containing three 24 bit registers, two for information and control and the third for testing. In this respect, the X-Rad was just another of the many Input/Output devices connected to the main computer.

Priority logic accepted asynchronous interrupts from up to eight sources including two quanta detectors, the four goniometer circles and two associated with the V-store. Interrupts could be prioritised and dealt with in around 1 microsecond allowing peak count rates of 1M quanta per second, assuming single detector operation. Average count rates were much lower, around 10k per second. When counting was in progress just two circles would be in motion, the *omega* and *twotheta*, at quite a slow rate, around 0.5 deg/second. At this speed the interrupt request rates associated with positioning average one every 10 milliseconds and these have minimal impact on peak counting rates. Of course even low priority interrupts must be dealt with in the same time as the highest to avoid potential loss of counts.

The Sequel

The Atlas on-line system worked well and productively for a number of years and benefited from direct digital interfacing between the diffractometer and Atlas. However, with only a small number of Ferranti Atlas computers in existence it did not provide a general solution which could be used to satisfy the increasing demand for automated systems. Around the time the first Atlas system was completed at Manchester new small, relatively cheap, minicomputers became available which could potentially be used to replace a lot of the special hardware with software. Hilger and Watts were keen to take advantage of this opportunity and one of the very first DEC PDP-8 was purchased. There are claims this was the fourth machine to be sold by the company. It was certainly very early days for DEC in the UK. I remember spending time at the UK headquarters in Reading, then bare-boarded space over a carpet shop in Castle Street, testing bits of software before our production machine arrived. A lot of the floor space was used to store machine manuals which were handed out at exhibitions as sales material. No glossy sales leaflets. One of the technical staff was Geoff Shingles who stayed with DEC as it expanded to be a very large operation in the UK.

As the PDP-8 had a short 12-bit word length double length working was needed for the circle position and detected quanta count registers. However, with some pre-scaling of the count rate, the machine was quite capable of satisfying the time constraints of the application. The diffractometer inputs were handled by the PDP-8's priority interrupt system, emulating the special hardware of the Atlas X-Rad. A bespoke operating system functionally replicated the X-Rad control hardware and also allowed background pre-processing of positional data. For this, software floating point functions were needed to achieve the necessary accuracy.

However, the PDP-8 certainly did not have the capability to do the processing of collected data and this had to be done off-line on another more appropriate machine. The standard input/output for small machines at that time was provided by the paper tape reader and punch options of the widely used Teletype keyboard and printer device. The initial advantage of using paper tape for input and output was its universality but apparently some later systems were adapted using digital interfaces to achieve more elegant solutions.

The Hilger and Watts PDP-8 system enjoyed considerable commercial success and was used quite widely in the UK, apparently until the 1980s, and abroad. One story suggested two systems went to the USSR but were never heard of again. In 1966 the company gained a Queen's Award to Industry for service to export and in 1968 a second Queen's Award for technical achievement.

Jon Cooper (Emeritus Professor of Structural Biology at UCL) has written a fascinating historical article, with lots of photographs, entitled *'Squaring the Blue Four-Circle'* (link at the end) which puts the PDP-8 Hilger and Watts system into context with other work at the time and preceding it from a user's perspective. It clearly references the Manchester input. Apparently, a system at the University of Oxford was not retired until 2007, although by then enhanced by computer upgrades.

Rounding off

The Atlas X-Rad system successfully demonstrated the principles of an automated on-line data collection system tightly integrated with a time-sharing computer. It was intensively used for diffraction studies for several years, fully exploiting the new capabilities of the Hilger and Watts four-circle diffractometer. It was ahead of its time in the sense that as it was very much a part of the Atlas system possibilities for replication were extremely limited and it never happened.

However, the parallel introduction and explosive growth of relatively cheap mini-computers, such as the PDP-8, made it attractive to design stand-alone systems which could be acquired much more easily by research laboratories. They still automated the data collection process but relied on links to other computers to do the more complex data processing of results. In today's world, networking allows easy interconnection and the paper tape transfers of the PDP-8 age are long gone.

Further information can be found in: *A small computer applied to real time data collection*, D. B. G. Edwards, K. F. Bowden, J. Standeven, O.S. Mills. Computer Bulletin, Vol 10, No 1 June 1966 and *An Operating System for a Small Computer providing Time-Shared Computing and Control Functions,* J Standeven, K F Bowden, and D B G Edwards, I.F.I.P. Congress, Edinburgh, August 1968.

Also, the relatively recent, article by Professor Jon Cooper of UCL, mentioned above, to be found in the International Union of Crystallography (IUCr) Newsletter (2020), Volume 28, Number 2: *'Squaring the Blue Four-Circle'*
https://www.iucr.org/news/newsletter/volume-28/number-2/squaring-the-blue-four-circle
The blue refers to the trade-mark Hilger and Watts colour for their scientific instruments. The article has internal links worth following too, including Wikipedia.