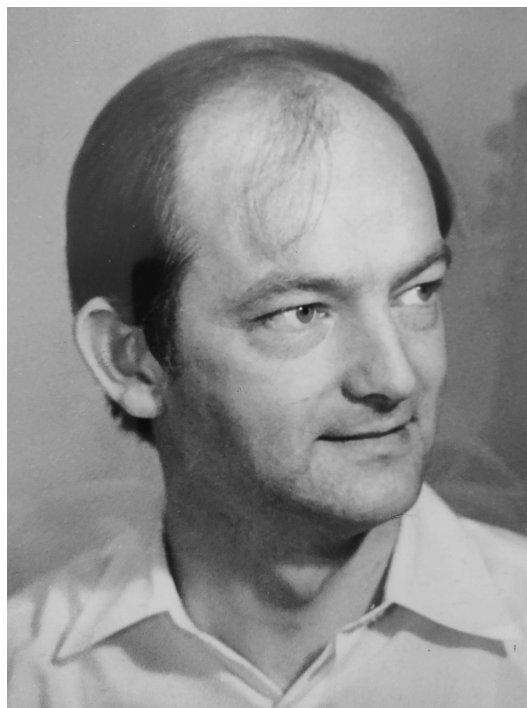


Peter Main (1939–2024)

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Peter Main, who died on 3rd November 2024, was an innovative scientist and a brilliant teacher. Since the 1960s, Peter had helped transform our knowledge of chemistry and biochemistry, by providing computer software which revolutionized chemical crystallography. He later worked on density modification algorithms which helped solve many protein structures, as well as inspiring others to push these methods further.

He was an outstanding teacher, always lucid and clear when explaining tricky crystallographic phenomena, and many of us who also worked in the field are deeply indebted to him for this.

Peter was born in the small Northumbrian village of Newbiggin-by-the sea, an idyllic spot on the Northumbrian coast. (This maybe helps explain the delight he felt when he could escape into the countryside.) However, he was destined for academia. He studied Physics at the University of Manchester Institute of Science and Technology, and proceeded to do a PhD with Michael Woolfson, a theoretical crystallographer who had made important contributions to the principles underlying phase estimation for structure-factor observations, already labelled as ‘direct methods for phase determination’.

Peter’s thesis covered more classical crystallographic material; he solved a 16-atom structure by Patterson methods and programmed various calculations, first in a language called Autocode, but later in the much more flexible Fortran language which would dominate early scientific software development.

After his graduation he spent time as a postdoc in Purdue, Indiana, USA, working with Michael Rossmann. Michael had helped develop mathematical methods to use the information present due to non-crystallographic symmetry in protein crystallography, and already saw that this could help refine phases for highly symmetric molecules such as

viruses once it could be precisely described. Peter contributed to solving this problem, both by developing the theory and programming the required software.

By 1967, Michael Woolfson had been appointed as Professor of Theoretical Physics at the newly established University of York. He invited his former graduate student, Peter, to join the department as a lecturer, apparently without needing to consult human resources or anyone else!

There followed a period of great creativity, culminating in 1971 with the release of the program *MULTAN*. *MULTAN* implemented a 'direct methods' procedure – assign phases to three reflections to define the crystal origin, select a few of the largest reflections and assign them random phases, then generate new phases for more reflections using the 'tangent formula'. The results were ranked by a range of figures of merit; the most promising sets were used to calculate maps, and if these showed a structure which made chemical sense, the trial was deemed to be a success.

For the next decade *MULTAN* was used to solve most small non-centrosymmetric structures worldwide. It was (and is) a prime example of good programming technique. The program was modular, meaning that, for instance, if a more sensitive figure of merit was discovered, it was simple to add it or replace existing ones. The crystallographic library routines were well designed, well documented and rigorously tested, functional for all space groups, and reusable in other applications. The results were clearly presented and for portability the programming language used was the most basic Fortran.

By 1971, York was recognized as one of the most active centres of direct methods development. Michael and Peter organized a number of very influential direct methods schools. The first, sponsored by NATO, gave a broad overview of the theory and methods of structure determination, and stimulated many students who went on to become leading crystallographic theoreticians themselves (Fig. 1). It was followed by many others – in Erice (1974), York (1975), Erice (1978) and York (1980).



Figure 1

The 1971 NATO School official photograph. Typically, given Peter's modesty, he cannot be identified here. Included in the front row are M. M. Woolfson, P. P. Ewald, D. Rogers, D. Viterbo and P. Beurskens. A. L. Spek is two rows behind the lady in the middle of the front row. W. Duax is behind Rogers.

Peter's lectures on direct methods were always beautifully organized. Whenever possible he was asked to open a session – he could make complex ideas seem comprehensible and set the context for new innovations.

During the 1980s, protein crystallographers were realising that although the limited data and poor initial phase estimates obtained for proteins could not yield images that showed individual atoms, their maps did possess other features, such as solvent boundaries, which provided information to improve the phase estimates (Wang, 1985). Michael and his Chinese colleagues were exploring these ideas, and by the late 1980s Peter and his research students Kam J. Zhang and K. Cowtan were providing software applying sophisticated density modifications in real space to perform direct-methods style phase improvement. The programs were distributed with the *CCP4* (Collaborative Computing Project Number 4) suite of programs (Winn *et al.*, 2011; Agirre *et al.*, 2023) and widely used (Main, 1990*a*, 1990*b*; Zhang & Main 1990*a*, 1990*b*). This led to fruitful collaborations between the physicists and the structural biologists based in York Structural Biology Laboratory (YSBL). SERC funded a collaborative project to assist the links, and the two groups worked closely together over the next decades.

Physics Review magazine was first conceived in May 1990. Several staff at York were particularly excited by the possibilities and submitted a proposal outlining a range of possible approaches to the design, content and overall philosophy of the new magazine. This proposal was successful and led to the establishment of a multidisciplinary editorial board based at York, whose joint efforts led to the first issue being circulated to schools in September of 1991. It was to be 'pitched at the



Figure 2

Peter Main in his later years.

middle-ability 16- to 17-year-old physics student, who has a reasonable grasp of physics at GCSE level, is in the process of getting to grips with some A-level or equivalent material and whose main interest is not necessarily in pure physics'. Over the next 24 years Peter submitted 125 articles to the magazine, on subjects ranging from surfing to music.

Peter expressed his love of the outdoors through cycling. He once told me (EJD) that he *always* cycled with a packed lunch because he did not like to leave his bicycle alone while he went into a cafe! In 1990, after a heart bypass operation a year earlier, he cycled the 1038 miles from Lands End to John O'Groats to raise money for a coronary support group. He was also a keen walker; in 1981 five members of the Physics Department bought Goose Howe, a cottage in the Lake District, and Peter had spent a week there just before he died.

He was passionate about music too, playing the church organ and Northumbrian small pipes. After his retirement the one place you could be sure to find him was at the keyboard in Heslington Church. Both enthusiasms informed his teaching –

he taught undergraduates about the physics of music, and published articles in *Physics Review* about the physics of cycling.

To sum up, Peter was a rock – always patient, always well informed, always willing to support his students and collaborators, modest to a fault and self-effacing, but always there when needed. We are all lucky to have had such a friend.

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