

Celebratory Symposium for MCP's 60th birthday

Community

in our field of science, in UK and Europe and Worldwide,

particularly Mike's contribution

from Volker Heine

First of all I give my heartfelt congratulations to Mike on his 60th birthday. All the talks today have borne testimony to his many contributions, and my thanks also go to the organisers.

My topic today is 'community'. We only have to look around this room to see what is meant by community in practice. In particular we see the wonderful work that has been achieved thanks to the close cooperative working together of that community.

Indeed the CASTEP community with its CASTEP Development Group and Tutorials for beginning users is part of a larger noticeable development since around 1980, illustrated by a little story. I was talking in mid or late 1990s with a friend on the Continent and a visitor from USA, and saying how building cooperation has made Europe now one of the leading areas in the world for electronic structure calculation, and our USA friend dug me in the ribs and said "Go on – THE leading area!"

However I just want to comment that it did not always come easily! High Energy Particle physicists work in armies with 1000 names on a paper, and astronomers and nuclear physicists and others hunt in large packs around their necessary large machines. One result is that Condensed Matter Physics has become the last refuge of the individualist! Just look around you in this room....!

Indeed there was a time in the late 1990s when I wondered how the working together would be carried forward in Britain. I was nearing retirement, and so were other UK leaders of such cooperation across Europe. Who were we in UK? Of course there were others, including Richard Needs in the Total Energy and Force Club mentioned today. But a lot seemed to rest on good Brit Walter Temmerman (from Belgium) and good British woman Dzikka Szotek (from Poland) and good Brit Balacz Gyorffy (from Hungary) and good Brit Volker Heine (from New Zealand plus German childhood)!

Well, I am personally very gratified how the next generation has in fact picked up the baton. We see it in this room revolving around CASTEP etc.; we see it in the Thomas Young Centre in London; we see it in CCP9 which I have been told is the only [original] CCP still in existence; we see it in the European Research Network 'Psi-k' centred on Daresbury; we see it in the Total Energy and Force Club which started in a discussion in a pub in Oxford; we see it in CECAM which started with chemical static and dynamic simulations with classical interatomic potentials but then merged with electronic structure interests after the Car-Parrinello paper; and we see it elsewhere. [Historical note – The CCPs were a major step in building cooperation. In 1978 the Cray 1S computer at Daresbury was the first supercomputer on this side of the Atlantic open to university researchers, and the CCPs were formed to develop computational science and publicise its use in the UK as a major expensive facility.]

I would like to set down explicitly the three principles that were the basis for cooperation in the Psi-k Network covering all electronic structure calculation. Firstly science matters more than anything else such as prestige, money, large groups etc. Secondly we tried to reach out to all researchers in our field, not just the substantial groups. One calculation is ultimately done by one person at one computer, and hence there were (and are) somewhat isolated individuals in small centres around Europe and in institutions focussed on various specialities. (I remember one person in a leading glass research institute bravely developing what our methodology might contribute there.) Thirdly Psi-k members created opportunities for young researchers to get into our field, some of whom are in this room today. Since ours was a new field of research, there were not necessarily opportunities in a student's own country. I am very touched how many of those 'young people', now perhaps with a few grey hairs (!), are continuing those traditions and garnering funding to keep Psi-k active. This is in trainings, workshops, summer schools, research conferences, the Psi-k Newsletter, and a big gathering of 'the whole family' (as Ole Andersen called us) every five years, the next one being in Lausanne next 14 – 17 September, with gatherings embedded within the European 'March Meeting' annually in Germany. Incidentally, Psi-k was initiated by Walter Temmerman in Daresbury around 1992 in response to a new EU initiative, and he pushed me into being the first chairman.

In this regard Mike Payne has been a leading contributor working for national and international cooperation in our field, as have many others in the group assembled here today. Leadership can come in different ways. One of them is organisational, such as through Psi-k, CCP9, the CASTEP community, etc. Here the wonderful CASTEP community is outstanding. A second way is to pioneer carefully thought out calculations with our methodology newly in different areas of science, which other people notice and then take further. Many of the papers presented today mention again and again Mike's contributions in this regard. Thirdly Mike's decision was pioneering to go for commercialisation of CASTEP when the Research Council refused to support its development beyond a couple of years or so. This was the first such code commercialisation in our field of science, born partly of necessity but also of far sightedness. I believe the huge developments we have heard about today could not have happened without the extra muscle from the commercial side. I mean the parallelisation to CETEP, the development of the 'order(N)' code ONETEP, the complete rewriting of the code at one point along the way, the supply of appropriately tuned pseudopotentials, the continuing extension of the code's capabilities and the expansion of the CASTEP community through about 40 Million dollars' worth of sales of the code, etc. etc.

I have a couple of little stories about the building of community along the way. The first is associated with the Total Energy and Force 'Club' as I call it. Around 1980 the UK Government established a few 'New Blood' lectureships in universities, because with the big university expansion and appointment of young academics in the 1960s there were no retirements and hence no opportunities for younger people around 1980. I applied for one in Cambridge specifically to develop in Britain ab initio simulations with pseudopotentials and plane waves, which was then still very new. This proposal did not get much traction in the Cavendish Lab, but the Research Council committees made the selection in that first year of the scheme, and funded my proposal. Richard Needs was appointed, and we sent him to Richard Martin in USA to learn about this method and bring it back to Britain. At that time there were only about five young people in Europe starting such work. One was Karel Kunc in Paris, who had also spent a year or two with Richard Martin, and had in fact written the code there, and brought it back about a year or two earlier. Matthias Scheffler had also returned from USA a year before, and similarly Sverre Froyen and another person in Copenhagen. That was all. Now remember what I said about

individualism. At that time the standard way would have been for everyone to write his own code, and develop his own pseudopotentials, etc. etc. etc. In addition a young person might have lecturing or other responsibilities. I remembered my supervisor, Professor Sir Nevill Mott once saying to me: "There is a great deal of research going on in our universities which is very important to keep staff and students intellectually alive, but its contribution to the furtherance of knowledge is practically zero." Quite!!! But I did not want us to do that kind of research! And with the highly competitive New Blood post, we had to produce! So after a conference in Oxford, this little group met and I said to them "You have not got a hope in hell of getting to the world forefront of research in the bad old way of going it alone. We have to cooperate!" Matthias in particular took note and then organised the first Total Energy and Force workshop in Braunschweig. Well, 'the rest is history' as people say, and the annual workshops still continue, now centred on the ICTP in Trieste.

My second story concerns Mike directly. In the early 1990s, it became clear that parallel computing was going to be the way of the future. And then it suddenly arrived on our doorstep! The High Energy Physics community wanted to do the first major Quantum Chromodynamics calculations and had their eye on a Meiko parallel computer. It would cost £1M, but the relevant committee of the Research Council only had £750K. At that time the chairman of the Research Council liked 'inspirational' funding, and decided that they should get 3/4 of a Meiko and that the other 1/4 should come from the physics and chemistry community. He also decided that its use should not be frittered away in a multiplicity of small individual calculations but should be devoted to an innovative project that would make a splash. But what project??? Now it happened that the industrial chemist Dominic Tildesley was on the relevant committee in the Research Council, and he said "Last month the cover of our chemistry magazine was devoted to the Car Parrinello method. So that is something which would be new to the UK and should have joint support from the physics, chemistry and materials science communities." The latter point was of course important with £250K at stake! So CP it was and a small group met in Oxford to plan it. But how does one parallelise electronic structure calculations??? Now you all know the answer but it was not obvious to us at that time. In the preceding years I remember some conversations at CCP9 meetings about parallelising electronic structure. Obviously one could parallelise on different k-points, but that didn't seem to get one very far, especially as one wanted to do larger systems. We were stumped, and went home from Oxford depressed with that £250K just out of reach!! But it focussed Mike's mind wonderfully, and at our next meeting he came up with the answer, which utterly stunned us. It is a good example of the difficulty of thinking a completely new thought that no-one in the world had ever thought before! We had always thought of a Bloch function as one entity, as it had always been throughout our lives in physics. Thus the UK Car-Parrinello Project became airborne, and the rest is history, as one says.