THE RISE OF SCIENTIFIC COMPUTING – A UK SUCCESS STORY

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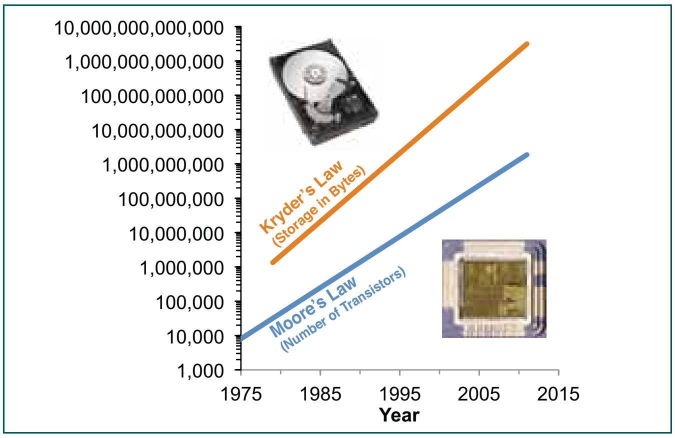
THEY JUST GET QUICKER AND QUICKER

Computer based, attention-diverting technologies, improve year on year. This is facilitated by a steady increase in 'computer power'. When and why that increase will end has been discussed endlessly for years, but the computers don't listen and continue to advance. Furthermore, that growth is not linear. There are various measures for the increase in computer performance. Two often quoted 'laws' are due to Moore and Kryder (actually neither are true laws but empirical observations). Both express improvement in terms of a doubling of performance over a time period.



A comparison of Moore's Law with Kryder's Law

Moore's Law counts the number of transistors on an integrated circuit – roughly, the more transistors, the more work that can be done. This number has doubled every 18 months, or by a factor of a thousand after 15 years. Kryder's Law considers the density of hard drives which equates to available data storage capacity. This doubles even quicker, every 13 months, or by a factor of a thousand after roughly 11 years. In my 30 years as a computational scientist, the capability of computers to deliver results has increased by a million, but for storing those results, by a factor of two hundred million! What have been the consequences of this explosion in capability and how has the UK exploited it?

THE AGES OF COMPUTING

1943 to 1970. The world's first programmable electronic digital computers were designed and built at Bletchley Park. Despite rapid improvements in performance, computers throughout this period were used as little more than automated slide rules. They did, however, allow theorists to turn their equations into self-contained computer code (programs) that released numbers to be translated into simple graphs and diagrams for publication. UK scientists were quick to realise the potential benefits and the University of Manchester became an early international centre of excellence. Since the equations purported to describe the way nature behaved, predicting things we could observe experimentally provided an acid test for the validity of those equations. Simulations were often most useful when the prediction did not match experiment because it implied that nature behaved differently to how we thought, which led to better understanding.

From **1970 to 1985**, more generic computer codes emerged where the given code could tackle a range of problems for the user community. For example, in the UK, codes were devised for biological systems such as protein interactions, for representing the laminar flow of liquids and gases for chemical engineering applications, and for predicting the outcome of collisions – from cars to atoms. Much of the pioneering work was carried out by Harwell Laboratory near Oxford as part of its atomic energy mission, where access to Cray supercomputers enabled simulations to be carried out which had more scientific impact.

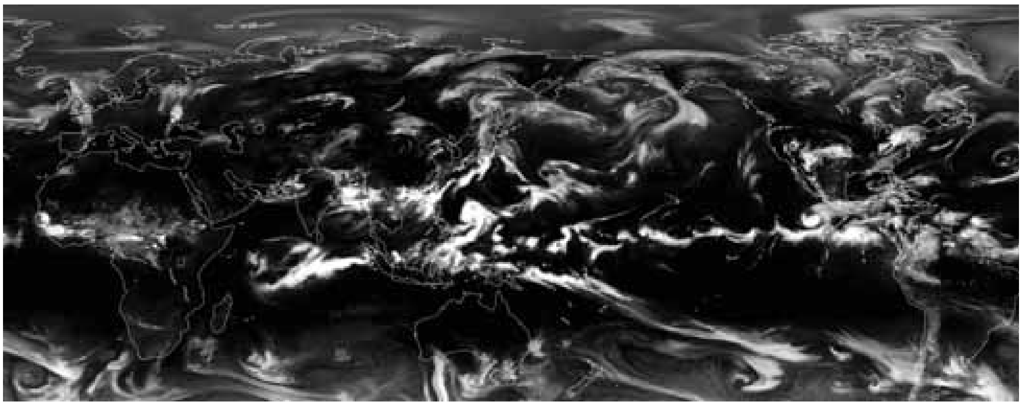
1985 to 2000 saw greater access to high end computer power, which meant much larger systems could be commonly tackled. The range of tractable physical and biological science problems also increased. Social scientists and economists also began to take advantage.

Now behaviours could be investigated that were beyond usual experimental techniques – for example, sub-atomic lengths, or on timescales of electrons transferring across simple molecules. During this time computer graphics started to become common. Post analysis of results now allowed secondary codes to draw the diagrams – essential given the larger data sets. It also allowed us to peek into time and length scales beyond routine observation. Experimental data was also being translated into graphics using computers, thereby providing high level understanding of measurements.

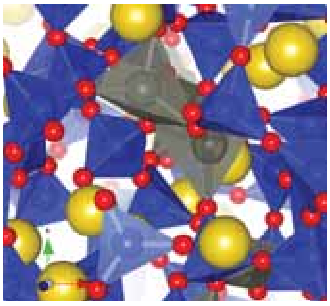
Since **2000**, computer simulation has really been a mainstream research tool. Increasing access to ever more powerful computational facilities is too tempting even for the most ardent experimentalist – especially in the UK, the majority of science and engineering students use some form of simulation tools to aid their research.

System sizes are much larger with a commensurate prediction of complex behaviour. This has delivered dramatic improvements in our understanding of physical systems. Prior to this we analysed systems that behaved in ways we expected. Now the codes and associated analysis tools were able to sift through data and simulate complex systems, such as the Earth's climate, by solving mathematical equations based on fundamental scientific properties, to reveal the consequences of this complexity and identify unanticipated behaviour. For example, simulating the turbulent flow of gases and liquids over many length scales enables us to predict weather patterns with kilometre precision.

The UK Met Office is a world leader in developing and applying these types of simulations but it requires a world class computing resource which can complete more than 1000 trillion calculations a second. We also maintained our world leading capability for predicting atomic scale systems – where graphics display millions of atoms engaged in fascinating and complicated gyrations, as shown below.



Met Office Climate Model simulation at 12km (credit: courtesy of Met Office)



Simulation of a zinc sodium silicate glass

UK prosperity benefited with many companies delivering simulation tools and analysis solutions to industries across the globe. Students also gained valuable skills that they took to related industries, especially the financial sector.

Most recently we have been occupied with the further democratisation of simulation. Now anyone can have a sufficiently powerful personal computer (PC) on their desk to carry out useful, if not cutting-edge, simulations. The UK is a leader in mobile computing with companies such as ARM and Imagination Technologies designing scalable semiconductor systems which provide opportunities to carry out simulations in different ways. The propensity to use simulation tools continues to grow. From the design of a next generation Formula 1 car to a new pharmaceutical, each begins with a foundation in simulation. Simulation is also a common tool for social scientists.

Looking forward, how different will those scientific simulations be to what came before? For a start, programs will act more autonomously, waiting for particular events or a stimulus before performing a simulation to compare with an observation. Already, enormous volumes of data are mined and selected using autonomous processes. Since programs are much more easily connected, the code itself will increasingly decide the next step. This adds to the complexity of the modelled systems and therefore the thirst for more computer power. One way to address that is by distributing tasks between machines using parallel computing protocols. This has been with us for quite a long time but parallel computing has been for the aficionado. We are currently developing codes that can do the heavy lifting for us, optimising the parallelisation on the fly.

The future of scientific computing is being supported though the Big data and energy-efficient computing initiative, one of the Eight Great Technologies. This will help the UK to maintain our lead and benefit from the decades of sustained academic activity. Amazingly, around 90% of all electronic data has been created in the last two years. The FCO is engaged with the burgeoning data science community's development of big data analysis tools and is working to embed the use of digital tools across every element of foreign policy work. The joint FCO-BIS Science and Innovation Network is busy helping to maintain the UK's high global profile, ensuring that UK scientists gain access to the best international networks.

Finally, I have no doubt that new generations of students will find new ways to use simulation to make exciting discoveries and in so doing will create new tools for industry and even new industries. This requires us to renew our digital resources and invest in the training of those new simulation scientists. Fortunately, the resource continues to evolve. The prediction of a plateau in computing performance is not supported by the observations – computers continue to get brighter and, unlike most of us, their memories are improving.