

<b>Institution:</b> University of Cambridge
<b>Unit of Assessment:</b> UoA9
<b>Title of case study:</b> CASTEP
<p><b>1. Summary of the impact</b> (indicative maximum 100 words)</p> <p>CASTEP is a parameter-free and predictive quantum mechanical atomistic simulation code developed by Professor Payne in the Department of Physics at the University of Cambridge. CASTEP has been sold commercially by Accelrys since 1995, with more than 800 industrial customers using the package. As part of Accelrys' Materials Studio, it can be used by non-experts to determine a wide range of physical and chemical properties of materials. Companies can thus perform 'virtual experiments' using CASTEP. As quantum mechanical simulations can be cheaper and more flexible than experiments, CASTEP invariably reduces costs and accelerates product development.</p>
<p><b>2. Underpinning research</b> (indicative maximum 500 words)</p> <p>CASTEP is based on the so-called 'total energy pseudopotential technique' which uses a plane wave basis set to represent the electronic wavefunctions, pseudopotentials to represent the ions and density functional theory to make the quantum mechanical calculations tractable. Total energy pseudopotential calculations had been applied to simple systems in the early 1980s but were restricted to small numbers of atoms from only a small part of the periodic table. Progress from the mid-1980s began to increase the capability of the calculations but (i) only one or two chemists in the world believed in density functional theory, (ii) there were concerns about the applicability of pseudopotentials to transition elements and (iii) it was not clear that the method could address complex problems. In 1991, Professor Payne (Department of Physics, University of Cambridge Assistant Lecturer from 1991, Professor from 2000), in collaboration with Edinburgh Parallel Computer Centre, ported his total energy pseudopotential code to parallel computers. Subsequent research exploited the increased computational performance of these systems and, particularly, the large amount of memory calculations that could be performed for larger and more complex systems. Thus, the concerns about the scope and capability of the total energy pseudopotential technique could be directly challenged through a series of innovative scientific applications. These applications not only proved that the criticisms of the total energy pseudopotential techniques were unfounded but also revealed the enormous scope of this approach. Amongst many other applications, these pioneering applications showed for the first time the capability of the total energy pseudopotential method to:</p> <p>perform dynamical simulations of chemical reactions [1];          determine absorption energies of molecules on transition metal surfaces [2];          model chemical reactions in extended solid state catalysts [3];          directly simulate experimental probes thus making a direct link between experimental measurements and underlying atomic structure [4].</p> <p>By 2000 the model for developing CASTEP through a combination of academic and industrial inputs (some coming from companies other than Accelrys) was failing. Like so many codes it had become bloated and undevelopable. Between 2000 and 2003, under a major research project, the code was completely re-engineered from scratch by the CASTEP Developers Group (CDG), with most the members of CDG being based in the Department of Physics in the University of Cambridge during this time (see details below). The code re-engineering made no re-use of existing code and was carried out using modern software engineering techniques to provide a robust, efficient, and portable code [5]. The aim of this research project was to provide a solid platform for development of new capabilities and functionalities for the total energy pseudopotential method. One example of this was the development of a suite of Nuclear Magnetic Resonance capabilities and the use of this to relate experimental NMR spectra to the underlying atomic structure – something not possible using experiment alone [6]. This research led to the development of an additional module CASTEP-NMR which is sold by Accelrys alongside the CASTEP package for those who want this additional capability.</p>

## Impact case study (REF3b)

Cambridge has provided the intellectual leadership for the creation and development of CASTEP. Throughout the relevant period the vast majority of the research underpinning CASTEP code development, including the key central modules, was done in Cambridge by a research group led by Professor Payne. Smaller contributions came from the UK Car-Parrinello consortium (UKCP), which also performed many applications of the code. Of the CDG, the following worked at the University of Cambridge Department of Physics as researchers/fellows during the census period (dates in brackets): Dr. Matt Segall (1997-2000, 2002-2007), Professor Chris Pickard (2000-2006), Dr. Matt Probert (1996-2000), Dr. Phil Hasnip (1996-2000 in the Department of Physics and then 2000-2005 in the Department of Materials), Dr. Jonathan Yates (2006-8). Members of the CDG not based in Cambridge: Professor Stewart Clark, University of Durham, Dr. Keith Refson, STFC Rutherford Appleton Technology Campus. Professor Francesco Mauri (Universite Pierre et Marie Curie, Paris) worked with the CDG on CASTEP-NMR.

### 3. References to the research (indicative maximum of six references)

\*[1] "Dynamics of dissociative chemisorption: Cl<sub>2</sub>/Si(111)-2x1" A De Vita, I Stich, MJ Gillan, MC Payne and LJ Clarke, *Phys. Rev. Lett.* **71** 1276 (1993). DOI: 10.1103/PhysRevLett.71.1276

[2] "Gradient corrections in density functional theory calculations for surfaces: CO on Pd(110)", P. Hu, D.A. King, S. Crampin, M.-H. Lee and M.C. Payne, *Chem. Phys. Lett.* **230**, 501 (1994). DOI: 10.1016/0009-2614(94)01184-2

\*[3] "Understanding the catalytic behaviour of zeolites - a first principles study of the adsorption of methanol", R. Shah, M.C. Payne, M.-H. Lee and J.D. Gale, *Science* **271**, 1395 (1996). DOI: 10.1126/science.271.5254.1395

[4] "Role of covalent tip-surface interactions in noncontact atomic force microscopy on reactive surfaces", R. Perez, M.C. Payne, I. Stich and K. Terakura, *Phys. Rev. Lett.* **78**, 678, (1997). DOI: 10.1103/PhysRevLett.78.678

\*[5] "First principles methods using CASTEP", S.J. Clark, M.D. Segall, C.J. Pickard, P.J. Hasnip, M.J. Probert, K. Refson and M.C. Payne, *Zeitschrift fur Kristallographie*, **220**, 567 (2005), ISSN 0044-2968

[6] "Theoretical investigation of oxygen-17 NMR shielding and electric field gradients in glutamic acid polymorphs", J.R. Yates, C.J. Pickard, M.C. Payne, R. Dupree, M. Profeta and F. Mauri, *J. Physical Chemistry A* **108**, 6032 (2004). DOI: 10.1021/jp049362+

\* References which best reflect the quality of the underpinning research.

### 4. Details of the impact (indicative maximum 750 words)

It is widely accepted that computation and simulation is a driver of economic growth. The most important requirement for industrial adoption of any simulation method is that the method must be accurate enough to be 'useful', essentially that it can be relied on when making decisions. This has always been the overriding factor in, leading provider of atomistic simulation software, Accelrys' choice of codes to support within its modelling environment as it has been determined to maintain its position at the 'high quality' end of atomistic simulations. CASTEP has had significant impact because it predicts physical properties to an accuracy of a few percent using no adjustable parameters and requiring no prior information about the system, thus clearly fulfilling industry and Accelrys' requirements for simulation codes. Accelrys' own success can also be attributed to the ease of use of its products. For instance, it was the first company to provide access to materials simulation methodologies through a graphical user interface. CASTEP is completely aligned with this philosophy, being the first quantum mechanical materials simulation code that truly abstracted all the complexity out of the calculations to make the methodology highly accessible. Given the combination of accuracy, predictive capability and ease of use that CASTEP provides, the final factor determining the level of industrial use, as with any simulation method, depends on its cost effectiveness compared to other methods for obtaining the same information. Continuing research has significantly decreased the computational costs of CASTEP calculations over and above that provided by Moore's Law, thus increasing the number of tasks that are most effectively assigned to CASTEP. Furthermore, the continuing decrease in the cost of computation means that even if a simulation method is not cost effective at a particular time it is likely to become so at some time in the future.

Quantum mechanical simulations using CASTEP have provided the ability to perform 'virtual'

## Impact case study (REF3b)

experiments on materials. However, there are many different types of materials and a vast range of physical, chemical and materials properties of interest involving a wide range of lengthscales and timescales. Therefore, simulation is not yet capable of replacing experiment to determine all materials properties of interest. Accelrys stresses just how much CASTEP offers in solving these classes of problems, by advertising the software suite as able to ‘*simulate the properties of solids, interfaces, and surfaces for a wide range of materials classes, including ceramics, semiconductors, and metals, with this premier density functional theory (DFT) quantum mechanical code*’. Such simulations enable customers to gain information about impurities in semiconductors, optical properties of materials, chemical reactions in catalysts, surface and bulk diffusion, refine atomic structures and generate the ‘experimental’ spectra associated with these structures.

The separate package CASTEP-NMR has provided is capable of generating the NMR spectrum associated with a model structure and thus the combination of experiment and CASTEP-NMR allows unambiguous determination of structures of crystals. This is particularly important in the pharmaceutical sector where a drug patent has to not only specify the drug molecule but also the crystal structure (the particular crystal polymorph) of the drug in the pharmaceutical product. CASTEP-NMR helps to identify the actual polymorph and, importantly, deviations in experimental data from that predicted. CASTEP-NMR is also used to identify low levels of other polymorphs in the product. If these other polymorphs are not patented then competitors may circumvent the patent by marketing the drug in the form of the non-patented polymorph.

The greatest impact of quantum mechanical simulations is often when they are used alongside experiment, as in the pharmaceuticals example above. For competitive reasons companies tend to be very secretive about their detailed use of simulation codes. Illustrative examples of the application of materials simulation approaches can be found in the IDC report “*Modeling and Simulation: The Return on Investment in Materials Science*,” and the Goldbeck Consulting report “*Economic Impact of Molecular Modelling*”. These reports mention many of the societal and economic benefits clearly provided by CASTEP including (i) efficiency: many different properties of many different classes of materials can be determined using a single piece of ‘apparatus’, namely a software package and computer; (ii) the broader exploration of materials solution space possible once simulation becomes significantly cheaper than experiment; (iii) projects which had stalled were restarted with information obtained from simulation and (iv) reduced time to market.

That CASTEP has proved to be exceedingly useful to industry is reflected in its use by more than 800 companies and its on-going sales in excess of £1million every year since 1998, with cumulative worldwide sales now over \$30million, demonstrating the value placed by commercial clients on access to the software. Sales over the audit period have been (US\$): 2008 - \$2,349,254, 2009 – \$2,067,239, 2010 - \$2,527,064, [9]. The IDC research [7] suggests that the return on investment in atomistic simulation is of the order of a factor of 7– which implies that the total economic impact of CASTEP is £hundreds of millions with benefits in many different sectors.

Accelrys has expressed its confidence in the importance of the CASTEP suite to the materials industry. With 830 unique customers, many of whom are household names (Boeing, Toyota, GM and DuPont for instance), the ability to make valuable predictions about new materials being used in new now ways offers huge scope to diverse industries to develop their product portfolio, or have confidence in the use of the materials in new applications. Product innovation has been enhanced very substantially by CASTEP’s use.

There are a number of published patents for materials or processes which have been designed partially based on CASTEP calculations. The number of distinct (i.e. not counting multiple filings in different regions) published patents that have used CASTEP as part of the inventive process in recent years are: 2008 – 12, 2009 - 5, 2010 -1, 2011 – 21, 2012 – 7 [10].

**5. Sources to corroborate the impact** (indicative maximum of 10 references)

[7] M. Swenson, M. Languell, and J. Golden, “Modeling and Simulation: The Return on Investment in Materials Science,” IDC, Jun. 2004. Can provide an electronic copy if needed.

[8] Goldbeck Consulting “The economic impact of molecular modelling”, 2012. Can provide an

**Impact case study (REF3b)**

electronic copy if needed.

[9] CASTEP and CASTEP-NMR Sales figures can be verified by the Senior Product Manager, Materials Studio, Accelrys

[10] Patent figures can be corroborated by a Goldbeck Consulting Ltd. patent report (held on file)