Institution: Loughborough University

Unit of Assessment: B10 Mathematical Sciences

Title of case study: Accelerating product development, reducing running costs and improving safety and performance in worldwide nuclear, chemical, automotive and semi-conductor electronics industries

Period when the underpinning research was undertaken: 2005 – 2009

Details of staff conducting the underpinning research from the submitting unit:

Name(s):	**Role(s) (e.g. job title):**	**Period(s) employed by submitting HEI:**
Roger Smith	Professor of Mathematical Engineering	1972 – present
Steven Kenny	Reader in Mathematical Sciences	2001 – present
Ed Sanville	Postdoctoral Research Associate	2006 – 2009

Period when the claimed impact occurred: 1st August 2013 – 2020

Is this case study continued from a case study submitted in 2014? N

1. Summary of the impact (indicative maximum 100 words)

Worldwide companies in nuclear, chemical, automotive, and micro-electronics industries regularly use an approach called 'density functional theory' (DFT) in the design and selection of new materials. To do this requires an efficient, reliable, and scalable method to analyse DFT output at the core of this process. Research undertaken at Loughborough University developed an algorithm for analysing DFT output that has been adopted worldwide. The beneficial impacts on the national and global commercial users of the algorithm have been: 1) accelerated product development and reduced research and development costs, 2) influenced the design and selection of new materials for improved performance and reduced operational costs, and 3) improved safety in the development and storage of nuclear materials.

2. Underpinning research (indicative maximum 500 words)

DFT is a method for solving the equations of quantum mechanics for the probability distribution of electrons in molecules and materials. It is used around the globe by industry and academia in the development of new materials and chemicals. Loughborough researchers have created a numerical method to partition charge distributions from DFT electronic structure calculations into atomic volumes, allowing for the visualisation of atomic bonding and for charge analysis. This methodology has become a standard analysis tool that works in conjunction with and has been incorporated into commercially available DFT software packages such as VASP, CASTEP and GAUSSIAN. For example, the algorithm is bundled with the VASP DFT code that has 15,000 organisational users worldwide. It is routinely used by both industry and academia to understand chemical and materials properties. This fundamental insight into such charge distributions has underpinned the computational design of new materials from over 50 companies.

The developed method uses Bader's charge analysis, which is a way of partitioning the charge between atoms from electronic structure calculations of molecules and materials, into atomic volumes based only on the electronic charge density. These atomic volumes are separated by zero flux surfaces, where the charge density is a minimum perpendicular to the surface. Finding these surfaces is challenging because the definition of the surface is non-local – one cannot determine if a single point is on a zero-flux surface without knowing the neighbouring points on the surface that define the surface normal. Our methodology provides an elegant solution to this

problem that is qualitatively different from previous approaches and is an order of magnitude faster and more accurate.

Before our work, to do a Bader charge analysis in an accurate and numerically efficient way, processing the output of DFT quantum chemistry packages, was inefficient and not robust. While the analysis of small molecules was possible, the complex atomic topologies found in material systems could not, in general, be analysed. Underpinning publications [**R1**] and [**R2**] describe numerical methods that not only do this accurately but also scale linearly with the number of interatomic surfaces in the system, so now large systems are feasible even on a small computer. This improved method is currently used in conjunction with all the widely used commercial quantum chemistry packages. The methodology described in [**R1**] and [**R2**] was devised in conjunction with Henkelman's group at UT Austin and the associated software is now publicly available from the UT Austin web site. The main coding was done by a postdoctoral researcher, Ed Sanville, at Loughborough under the supervision of Prof. Smith and Dr Kenny. Importantly, the work at Loughborough identified an orientation bias in an earlier algorithm and the collaborative work described in [**R1**] and [**R2**] removes this bias and is now the established method for doing Bader's analysis in materials.

An additional application of the Bader method allows the potential energy in a quantum system to be allocated to an atom. In a quantum description of a solid, the concept of a potential energy per atom is not defined. Reference [**R1**] uses the Bader charge allocation to define a potential energy per atom in a quantum system in a unique way, which can then be used to accurately parameterise classical potential functions, thus allowing computation for large systems of atoms beyond the scope of numerical quantum calculations.

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

[**R1**] Sanville, E., Kenny, S.D., Smith, R. and Henkelman, G., *Improved grid-based algorithm for Bader charge allocation*, J. Comp. Chem. **28**, 899-908 (2007), DOI: 10.1002/jcc.20575

[**R2**] Tang, W., Sanville, E. and Henkelman, G., *A grid-based Bader analysis algorithm without lattice bias*, J. Phys.: Cond. Matt. **21**, 084204 (2009), DOI: 10.1088/0953-8984/21/8/084204

Papers [**R1,R2**] were published in the peer reviewed leading academic journals and were funded by a £1.3m competitively-awarded peer-reviewed EPSRC grant (Title: "A multiscale modelling approach to engineering functional coatings" EP/C524322/1, 01/10/2005-30/09/2009).

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

The algorithm for performing the Bader charge analysis [**R1,R2**] has numerous industrial users worldwide, via a **pathway to impact** comprising a website that hosts the open source code [**S2**]. The code has been widely downloaded (there are over 200 downloads of the source code plus around 500 downloads of the compiled binary typically each month). Each of the two underpinning research papers [**R1,R2**] has achieved 1399 and 2787 (Web of Science) citations respectively in the current REF period (2014-2020), including citations by researchers from over 50 companies from a range of different industrial sectors including chemicals (Dow, BASF, Air Products, PraxAir, Bosch, Shell, Baker Hughes, Petrobas), vehicles (Daimler, Toyota, BMW, Mitsubishi, Nissan, GM, Daihatsu, Volvo, Subaru, Saic), microelectronics and semiconductor industries (GE, IBM, GlobalFoundries, Samsung) [**S5**]. The specific areas of impact in the nuclear, chemical, and sustainable technologies companies are described below:

Impact 1: Accelerated product development and reduced research and development costs

The Atomic Weapons Establishment (AWE) is the organisation responsible for the design, manufacture, and support of warheads for the UK's nuclear weapons. They used the Loughborough Bader charge analysis code in their work to understand the long-term storage

behaviour of oxides of radioactive elements, including Np, U and Pu, from which the warheads are made. Their As their Deputy Chief Scientist Norman Godfrey writes reported,

> "I am able to corroborate the significant impact of the Bader charge analysis code" which "was incredibly useful to us in the investigation of hydrogen adsorption on a range of actinide oxide surfaces where the actinides investigated included Np, U and Pu." [**S3**]

He also says that their use of the Loughborough code

> "has important implication for understanding long-term storage behaviour of these materials" … "Understanding actinide materials and the hydridising process is a key focus for AWE and the ability to investigate this process in silico ahead of experimental investigations enables a more focussed programme of work to be undertaken and hence maximise research outcomes." [**S3**]

Thus, the use of the Bader charge analysis code has enabled them over the impact period to save significant time and money as they discharge their duty to the UK.

In a similar way, Johnson Matthey PLC, a British multinational specialising in speciality chemicals and sustainable technologies, operating in over 30 countries, with annual sales of £4.2 bn and having >15,000 employees worldwide, used the Loughborough code to develop

> "new materials for new product developments in e.g. rechargeable battery for electric vehicles, fuel cells and other key sustainable technologies across a wide range of application sectors" … "The main impact of the research translated into an **improved development time for new products and processes**. The insight given by the Bader charge analysis code enables us to select in silico new potential materials faster and with more confidence for experimental testing" … "A good indicator of the importance and benefit it brings to JM is the fact that **we now use it in approximately 30% of our projects**" [**S4**].

International reach of our code can be seen for example from its use by Murata Manufacturing Co. Ltd (a Japanese manufacturer of electronic components). Their Senior Researcher, Yasuaki Okada, wrote that

> "[t]he theoretical prediction was utilized by R&D members to clarify promising cation species in electrolyte and we could reduce the number of experiments for the development of this electrochemical capacitor products" [**S5**].

A similar statement is made in a letter of support from Umicore Denmark [**S5**].

Impact 2: Influenced design and selection of new materials for improved performance and reduced operational costs

At the Government of India Bhabha Atomic Research Centre (BARC) new materials for thorium fuel based nuclear reactors are developed. The Loughborough Bader charge analysis code was used as an integral part of their work, in a manner typical of the ways the code is applied in new materials development. They tested various fuels containing compounds of thorium, using the code to identify the interaction between gases such as Helium produced in the fuel rod by the fission, which then affects over time the structure of the rod, leading to swelling and reducing its lifespan. In their letter of support [**S6**], Dr Arya, the Head of the Glass and Advanced Materials Division writes that the freely downloadable Loughborough code was

> "used in conjunction with quantum mechanical software packages [and] was incredibly useful to us". He then goes on to write "The impact of the research was therefore a change in the design of the composition of the fuel to minimise adverse effects of fission gases and frequency of refuelling, thereby saving significant amounts of money."

The same benefit of influencing design and selection of new materials is articulated by Johnson Matthey PLC [**S4**] which says the Bader code "allows us to guide, make and test different materials". Similarly, in their letter of support, Murata Manufacturing Co. Ltd [**S5**] state that the code "was utilized by R&D members to clarify promising cation species in electrolyte" also shows this impact.

Also, from the publications that cite the use of the Bader code, one finds more examples of the code influencing the design and selection of new materials by non-academic users. For example, BASF, the German multinational chemicals company (the largest chemicals producer in the world), rejected a potential cathode material for lithium ion batteries after using the Bader code [**S5**]. Similarly, CNEA, the main nuclear energy research laboratory in Argentina, used the Bader charge methodology to help assess the use of ThC as a potential material for future fission reactors [**S5**].

Impact 3: Improved safety in the development and storage of nuclear materials

The Government of India Bhabha Atomic Research Centre (BARC), who used the Loughborough code in their development of new materials for thorium fuel based nuclear reactors, emphasized in their letter of support [**S6**] the impact on **safety** that our research has had – and will continue to have in the future – writing that

> "the modelling involved in getting the correct fuel design is absolutely crucial which will drastically reduce the financial burden and will provide safeguard against any fatal nuclear accident. We will continue to test new fuel compositions to determine the optimum and the Bader charge analysis will continue to play a crucial role in this design process."

The Government of India Bhabha Atomic Research Centre [**S6**] also commented that "by proper designing, the integrity of nuclear fuel can be maintained over a longer time scale with all safety features intact."

Similarly, the Atomic Weapons Establishment (AWE) [**S3**] emphasized the safety impact related to the long-term storage of nuclear materials from their research using the Loughborough code.

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

[**S1**] Statement of support from VASP Software GmbH, dated 13th May 2020

[**S2**] Statement of support including link to software from UT Austin, dated 18th Oct. 2020

[**S3**] Testimonial letter from the Atomic Weapons Establishment (AWE), dated 25th Nov. 2019

[**S4**] Testimonial letter from Johnson Matthey PLC, dated 3rd Sept. 2020

[**S5**] List of publications from non-academic users of the Loughborough code and letters from some of them, dated Aug. 2020

[**S6**] Testimonial letter from the Government of India Bhabha Atomic Research Centre (BARC), dated 28th Nov. 2019