Institution: Swansea University
Unit of Assessment: 15 - General Engineering
Title of case study: The economic benefits of finite element/discrete element analysis when applied to industrial problems involving coupled field and multi-fracturing phenomena

1. Summary of the impact

Computational research work at Swansea concerned with finite element/discrete element analysis, has made a profound impact on the solution of industrial problems. The development and implementation of novel computational algorithms and their subsequent application to leading edge engineering and scientific problems has been effected through the commercial software system ELFEN, developed collaboratively with Rockfield Software Ltd, a spin-out company from Swansea University. ELFEN has enabled the company to expand through the development of an international reputation as a leading provider of computational technology to the defence, manufacturing, oil recovery, mining and other sectors. Specific examples of economic benefit described in this case study are (i) design methodology for weight reduction in glass container production resulting in significant energy and CO_2 emission savings and (ii) computational modelling of rock blasting operations leading to substantial economies in the mining industry.

2. Underpinning research

This impact case is based on a programme of research work undertaken over the last two decades focussed on the development of computational techniques, encompassing fundamental theoretical advances, the development and implementation of novel computational algorithms and subsequent application to leading edge engineering and scientific problems. The work was lead by Prof. D. R. J. Owen and Prof. D. Peric, with substantial contributions also made by Prof. Y. T. Feng, Prof. E. A. de Souza Neto, Dr. W. Dettmer (Senior Lecturer) and Dr. C. F. Li (Senior Lecturer), all of whom have been academic staff members at Swansea University throughout this REF appraisal period.

The thrust of the research has been directed at the numerical modelling of, firstly, the plastic deformation of solids under large strains, followed by the introduction of material damage and the ultimate development of a multi-fractured state, leading to a particulate system. Computational treatment necessitates a blend of continuous and discrete computational processes. Modelling aspects related to continuum problems include the development of advanced constitutive models, element technology for near-incompressible deformation, continual updating of the mesh (adaptive mesh refinement) and damage modelling for prediction of the onset of fracture [R2, R3, R6]. With the development of fractures, the domain becomes discontinuous in nature and further computational issues include strategies for discrete crack insertion that preserve the system energy, continual remeshing to accommodate the fracture distribution and global search algorithms to monitor contact of fragments in the resulting particulate system [R1, R4].

In several applications of engineering relevance involving multi-fracturing and/or particulate media, the behaviour is governed by the presence of an additional phase, either gaseous, liquid or both. Solution strategies that have been developed for such problems include coupled approaches for problems involving explosive detonation and progressively fracturing rock, and the integration of Lattice Boltzmann procedures for fluid modelling with discrete element approaches to solve problems related to particle transport, heat transfer in moving particle systems and segregation problems in multi-scale particle flows [R5].

The above developments form a computational technology platform, incorporated within ELFEN, for the solution of a range of multi-physics problems involving nonlinearly deforming and multi-fracturing materials that is highly innovative, world leading and applicable to large scale industrial problems. **ELFEN is a unique computational system which, to date, has no major commercial competitor and has enabled Rockfield to become an international leader in the provision of computational modelling services to several major industrial sectors.**

3. References to the research

The research has led to a substantial body of funding and publications and has been acclaimed as pioneering and internationally leading, being recognised by awards to the participants in the form of international prizes and honours (FREng, FRS, Koiter & Gauss-Newton Medals, Honorary Doctorates by University of Porto, ENS Cachan & UPC Barcelona, Foreign Membership US

National Academy of Engineering & Chinese Academy of Sciences), invitation to deliver named & plenary lectures, invitations to be editors of prestigious international journals (Int. J. Num. Meth. Engng., Arch. Comp. Mech. Engng., etc.) and to undertake collaborative work with leading international research institutions (Tsinghua, MIT, UT Austin, LNCC-Brazil, UPC-Barcelona, etc.). Selected publications and grants directly relevant to the impact claimed are provided below *(all Swansea authors are in bold type).* R1, R2 and R6 best represent the quality of the research.

Publications

R1. A. Munjiza, **D. R. J. Owen** and N. Bicanic, A combined finite/discrete element method in transient dynamics of fracturing solids. Int. J. Engng Computations. 12, 145-174, 1995. *(A well cited paper (>200 Google Scholar) presenting the initial concepts of the multi-fracturing approach)*. DOI: 10.1108/02644409510799532

R2. **D. Peric** and **D. R. J. Owen**, Finite element applications to the nonlinear mechanics of solids. In: Reports on Progress in Physics, Institute of Physics, 61/11, 1495-1574, 1998. *(A paper in a high Impact Factor journal (13.2 Thomson Reuters) invited to summarise the pioneering work of the authors – not a review paper).* DOI: 10.1088/0034-4885/61/11/002

R3. F. M. Andrade Pires, **E. A. de Souza Neto** and **D. R. J. Owen,** On the finite element prediction of damage growth and fracture initiation in finitely deforming ductile materials. Comp. Meth in Appl. Mech & Eng. 193, 5223-5256, 2004. *(A paper providing a theoretical foundation for the computational treatment of fracture).* DOI: 10.1016/j.cma.2004.01.038

R4. P. A. Klerck, E. J. Sellers and **D. R. J. Owen,** Discrete fracture in quasi-brittle materials under compressive and tensile stress states, Comp. Meth in Appl. Mech & Eng. 193, 3035-3056, 2004. *(A fundamental computational and theoretical treatment of multiaxial fracture in rocks).* DOI: 10.1016/j.cma.2003.10.015

R5. **Y. T. Feng**, K. Han and **D. R. J. Owen,** Coupled lattice Boltzmann method and discrete element modeling of particle transport in turbulent fluid flows: Computational issues, Int. J. Num. Meth. In Engng., 72, 1111-1134, 2007. *(A first paper in a series of publications integrating particulate and multi-fracturing solids with a range of coupled field effects).* DOI: 10.1002/nme.2114

R6. **E. A. de Souza Neto, D. Peric and D. R. J. Owen**, Computational Methods for Plasticity: Theory and Applications, John Wiley, 2011. *(This 800 page text on non-linear computational modelling is a leader in the field and brings together the research summarised above).* DOI: 10.1002/9780470694626

Research Grants

The underpinning research was funded by a total of 14 EPSRC grants, including the following:

G7. **GR/N21604/01 D. R. J. Owen & D. Peric.** An integrated simulation approach to the design of shaped can manufacturing processes. **20/07/00-19/07/03, £203,473** *(Focused on the development of large strain, elasto-plastic computational methods for advanced constitutive models, with application to real case industrial forming).*

G8. **GR/R87222/01 & GR/R87239/01 D. R. J. Owen & Y. T. Feng** Experimental/computational approaches for evaluating dynamically loaded reinforced concrete structures**. 01/08/02-31/12/05, £379,321** *(Directed at the development of computational dynamic impact simulation techniques for multi-fracturing solids, with experimental validation).*

G9. **GR/S04987/01 & EP/C518721/01 D. R. J. Owen & E. A. de Souza Neto.** Numerical modelling and analysis of fractured rock mass strength and deformability. **19/05/03-30/04/08, £218,891** *(Focussed on the development of computational capabilities for predicting rock mass strength in real mining situations).*

G10. **GR/R92318/01** (Platform Grant) **D. R. J. Owen, D. Peric, Y. T. Feng & E. A. de Souza Neto.** Computational strategies for large scale discrete systems and multi-fracturing solids. **01/01/03-31/12/07, £393,136** *(Aimed at the development of a comprehensive computational framework for the treatment of industrial scale problems involving particulates and large fracture systems).*

4. Details of the impact

The research work summarised in Section 2 forms the core technology employed in the commercial software system ELFEN developed by Rockfield Software Ltd., with extensive and continuous collaboration with the university. Rockfield is a spin-out company created with the aim of transferring the high quality computational modelling research of the internationally renowned numerical group at Swansea University to the commercial sector. The company has expanded to over 30 personnel, with over two thirds of the staff possessing Ph.D. degrees, making the company a significant employer of high technology graduates in the Swansea area and a valued contributor to the local economy.

Rockfield is internationally recognised as a leading provider of computational services to both SMEs and world-wide conglomerates and has, through the research support provided by the university, over the years built strong relationships with many of the world's foremost companies including; Unilever, IPGR, DSTL, Corus, Proctor & Gamble, Devonport Marine Ltd., Rio Tinto, BP-Amoco, Chevron, Shell, Exxon Mobil, Total-Fina-Elf, Miningtek, Orica, Anhauser Busch and Los Alamos, Sandia and Lawrence Livermore National Laboratories.

The importance of ELFEN to the success of Rockfield is evidenced by the granting of the Queen's Award for Innovation to the company in 2002 and 2007. In each case the award was granted for developments based on the ELFEN code, which indicates the extremely high level of impact of the technology on industrial and scientific innovation. Additionally, the prominent involvement of Rockfield in the mining and minerals recovery sector lead to the formation of Rockfield Technologies Australia, based in Townsville, Queensland to support these activities and the company currently employs ten R&D engineers.

The industrial impact has been made both through use of the methodology by Rockfield to develop its strong position within the computational modelling industrial community and by end use of the ELFEN system by the company's clients. Selected significant industrial contributions that have taken place during the REF reporting period 2008-2013 are summarised below:

Impact 1. Savings achieved by improvements in glass container production. Widely used in food and beverage packaging, glass containers account for 8% of the global packaging market, and are readily recyclable. Glass containers are made from sustainable raw materials (sand, soda ash and limestone) and mass produced through fully automated energy intensive forming processes. The primary energy demand (MJ/Kg glass) for production is estimated at 6.6, and the global warming potential (Kg CO_2/Kg glass) as 0.4. The EU annual production output alone is 22M Tonnes and therefore, the need for reducing the weight of containers is pressing, creating a rapidly growing demand for container specific optimization of glass forming processes. Computational simulation has proven to be an unrivalled tool for quantitative analysis of the complex multi-physics process involved in glass forming and a comprehensive version of ELFEN has been developed which can accurately simulate all major forming processes: blow-blow (BB), press and blow (PB) and narrow neck press and blow (NNPB). *"ELFEN-GD has permitted a 10-25% weight saving over traditional design methods and is widely accepted by glass manufacturers as a valuable design tool, with some 50 licences being employed worldwide"* [Managing Director, Rockfield Software Ltd.]. Among the principal users are Gallo Glass, USA, who manufacture 1 Billion bottles p.a. (~0.5M Tonnes of glass), Vidrala S.A., Spain who have a production capacity of 1.15M Tonnes (producing 3.3 Billion containers p.a.), with an annual turnover of £416M, and San Miguel Malaysia with a net annual income of US$207M. Vidrala state *"The computer simulation system ELFEN-GD has proven to be an invaluable tool for the design of forming processes for a wide range of our glass products. It is difficult to provide an accurate quantitative measure of the design improvements brought about by use of ELFEN across the range of our products, but it is estimated that lightweighting savings of around 10-15% have been achieved overall"* [Responsible Process R&D, Vidrala, S.A.]. With 50 licence users, it is conservatively estimated (accounting for their varying sizes) that these companies annually produce ~12M Tonnes of glass containers. ***Given a minimum 10% weight reduction brought about by ELFEN computational design (Rockfield and Vidrala support letters), this represents an annual primary energy saving of 14x10^6 GJ (~£70M p.a.) and CO_2 emission savings of ~ 0.5M Tonnes*.**

Impact 2. Savings in mining operations through explosive blasting simulation. Australia is the world's fourth largest coal producer and in 2010 produced 449M Tonnes of coal (export value ~

£35Bn). The efficiency of mining operations crucially depends on the development of explosive techniques that can control the fragmentation process to eliminate the need for secondary blasting of large particles and do not produce fine particles that deteriorate the quality of the mined material. Orica, which is the principal explosives manufacturer in Australia and whose turnover in 2012 was A$6.7Bn (£4.1Bn), have principal clients such as international companies BHP Billiton, Anglo American, Rio Tinto, and Xstrata who play a prominent role in extraction. Orica *"recognise ELFEN as the best and indeed the only tractable means by which we would be able to attempt to simulate blasting from the detonation phase to the bulk motion and settling phase, and today ELFEN is the mainstay of our modelling service to the mining industry. We have had unparalleled success using ELFEN to assist mines by simulating an extensive range of blasting scenarios. Orica management and our mining customers have long recognised the potential and value of such modelling and it is now seen as a serious, bone fide and valuable resource* ***with a potential estimated return of around A$30M over five or six years. In one blast in the Hunter Valley ELFEN saved one to two million dollars - we have used ELFEN to show how to achieve that on several occasions".*** [Senior Research Associate, Orica]

5. Sources to corroborate the impact

The ELFEN system is used by a range of SMEs and multi-national corporations world-wide. Principal sectors in which the company is involved include: (i) Defence applications involving explosive and impact conditions, (ii) Deep level mining and other minerals recovery operations, (iii) Oil recovery operations and resource prediction, (iv) Failure prediction for structures under seismic or blast loading, (v) Industrial forming processes for glass, plastics and metals and (vi) Food technology processes. Corroboration of the crucial contribution of the ELFEN system to allow Rockfield to be highly competitive in these areas is provided by the Managing Director, Rockfield Software Ltd.

With regard to the specific applications outlined in Section 4, the weight savings provided by use of the ELFEN-GD system in the design of a wide range of food and beverage glass containers is corroborated by the Managing Director, Rockfield Software Ltd.

The benefits of the software design system to individual end licence users is supported by a statement from the Responsible Process R&D, Vidrala S.A.

For the simulation and design of mine blasting operations, a Senior Research Associate of Orica, Australia testifies that the ELFEN multi-fracturing modelling capability is crucial to their mine management procedures and quantifies the benefits achieved.