The Economic Impact of Materials Modelling

Indicators, Metrics, and Industry Survey

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Executive Summary

In the framework of the European Materials Modelling Council (EMMC) and the International Materials Modelling Board (IM2B), the impact of materials modelling on the manufacturing industry has been analysed. At the core of the report is an industry survey conducted during 2015 that provides corroboration for the indicators of research and development (R&D) process improvements found in earlier studies and new data relevant for quantitative economic analyses.

The survey is set in the context of an outline of metrics and methodologies that can be used to quantify the economic impacts of materials modelling from a variety of perspectives including R&D and industry stakeholders and society at large. At the micro-economic level, performance indicators include financial metrics such as net present value, return on investment (ROI), and internal rate of return. Where sufficient data are available, micro-economic analyses could be extended to a more in depth cost benefit analysis. Finally, macro-economic modelling methodologies can be used to model the wider impacts of the integration of materials modelling into the production function of various industries. Since materials modelling is a potentially disruptive technology, macro-economic impact assessment will likely require dynamic simulation models, which are scenario specific and necessitate someone with a high level of both problem domain knowledge and modelling domain knowledge.

Research impact is reviewed briefly based on bibliometrics, case studies, peer review, and economic analysis [3] using evidence gathered for a previous report [4] as well as the recent UK Research Excellence Framework [5], which includes 15 cases involving materials modelling.

The study also investigates how materials modelling impacts the industrial R&D process and outlines the value and potential of materials modelling for industrial research and innovation, competitiveness, and profitability using examples from materials industries based on recent Integrated Computational Materials Engineering studies and a Computer-Aided Drug Design study, which demonstrated the usefulness of defining a performance metrics for a modelling function in an industrial R&D organisation.

The survey analysis was based on information provided by 29 companies covering a wide range of sizes and industry sectors and an even distribution in terms of types and scales of modelling. The qualitative benefits identified in the responses were categorised into the following Key Performance Indicators: More efficient and targeted exploration; Deeper understanding; Broader exploration; R&D strategy development; Source of property data; Trouble shooting; Performance optimisation; Intellectual property protection; Value chain benefits; Improved communication and collaboration between R&D and production; Upscaling and market introduction as well as marketing benefits.

On a quantitative level about 80% of companies reported innovation accomplishment, 60% cost savings, 35% job creation, and 30% revenue increase due to materials modelling. A wide variety of project sizes are represented, with total materials modelling investment (covering staff, software and hardware) ranging from €45K to €4M (average €1M, median €½M). Staff was the largest cost factor: the ratio of staff costs to the median cost of software and hardware, respectively, is 100/20/6. Cost savings due to the materials modelling project ranged from €100K to €50M (average €12M, median €5M). The ROI, determined by the ratio of revenue generated and investment in modelling, ranged from 2 to 1000. Removing the largest and the smallest values yields an average ROI of 8. A trend for ROI to grow more than linearly with investment in modelling was found.

Introduction

The introduction of any new technology or product has both costs and benefits. Historically, new opportunities, such as the locomotive or the introduction of the modern computer, provided long-term improvements in socioeconomic welfare but came with short term job casualties as populations worked to retrain and move people from areas that were structurally no longer required into areas of new or increased demand. Joseph Schumpeter coined the phrase "creative destruction" (or the "perennial gale of creative destruction") in his book *Capitalism, Socialism, and Democracy* [1] to describe the constant economic turmoil that ultimately leads to better jobs, better products, and higher standards of living in capitalist societies.

Materials modelling and the resulting advances in materials and products manufactured from these materials have the potential to significantly impact both the economy and society in a variety of ways. Impact is (obviously) a question of perspective, and so are the indicators and metrics that go along with that. The aims of this study are to investigate how materials modelling impacts the industrial research and development (R&D) process and to understand the value and potential of materials modelling for industrial research and innovation, competitiveness, and profitability. This effort includes gathering success stories and case examples involving materials modelling in academia and industry and analysing them to improve the understanding of the benefits of using materials modelling, as well as determining quantitative relationships between the investment in materials modelling and economic advancements such as additional revenue, cost savings, and job creation.

The first part of the report includes a general overview of the various types of impacts that could result from the use of materials modelling and a discussion of methods that exist for quantifying these impacts. Economic impacts are discussed with respect to a variety of time scales, geographic regions, and stakeholders.

In the second part, the wide range of impacts related to materials modelling research are discussed. Specific examples of impacts and impact evaluation methods discussed include bibliometrics, human capital impacts, macro-economic impacts, and evidence from the United Kingdom's Research Excellence Framework.

In the third part, indicators and potential impact metrics of particular interest to industry stakeholders are discussed. Evidence from previous studies of the materials modelling and integrated computational materials engineering (ICME) sectors are reviewed as well as a study considering how modelling as an organisational function in industry can improve its impact.

In the fourth part, a survey of manufacturing organisations is presented, providing corroboration for the indicators of R&D process improvements found in earlier studies and new data relevant for quantitative economic analyses.

1. Impacts of materials modelling

Current and future advances in the fields of computational modelling and materials science will undoubtedly lead to a variety of impacts of various types at various scales over an extended time horizon. There will be economic impacts associated with R&D spending, demonstration projects, and the deployment or availability of new software, new modelling techniques, new materials, and new products fabricated with these materials. The impacts will affect society on a variety of scales including the individual software, model, or material developers, the software design and materials manufacturing industries, and the economy as a whole. Also, the impacts will likely be different at various geographic scales, e.g. local, national, regional, and international. There is also the potential for these technologies and the materials and products they result in to bring about broader societal impacts as well including, but not limited to, impacts on environmental emissions, waste production, natural resource depletion, innovation, economic development, quality of life, etc.

A general description of the indicators, metrics, and methodologies that have been used to quantify the direct and indirect economic impacts of materials modelling are discussed below in terms of micro-economic impact assessments that analyse the impacts of materials modelling on a specific business or industry and macro-economic impact assessments that measure the impacts of materials modelling on the economy as whole. Additional detail on metrics and methods of particular interest to industry stakeholders are discussed in more detail in section 3.

Micro-economic impacts

Individual companies often find it necessary to provide a business case for investments in materials modelling. Also, developers of models or specific software packages find it necessary to determine the economic benefits of their particular model or software in order to justify its use within industry. In such cases, the derivation or calculation of financial metrics or indicators such as net present value (NPV), return on investment (ROI), and internal rate of return (IRR) are often a starting point for a more in-depth micro-economic assessment of impacts.

Analysts can also attempt to quantify the direct impacts on output, revenue, employment, and income that might result from new or increased investment in materials modelling efforts. Direct impacts for a particular company or industry might include savings on the costs of experiments, faster turnaround time on the development of new materials, increases in employment and income related to materials modelling, etc. Companies or funding agencies might also be interested in the assessment of changes in these variables that would result from the availability of materials produced with the aid of materials modelling. Oftentimes, model, software, or materials specific impacts related to output, revenue, employment, and income can be derived for use in business case development.

When more detailed data are available, cost benefit analysis can also be used to assess the total impact of a specific model, software, or material. Analysts could examine the costs (both direct and indirect) of the model or software along with the potential benefits (increases in revenue, employment, income, and any other non-economic impacts) to support the decision making process on a variety of levels.

Macro-economic impacts

Macro-economic impact assessment tools can be used to determine the impacts of materials modelling on the economy as a whole in terms of employment, income, and gross domestic product (GDP). Similar to the desire of a company to provide a business case for investments in materials modelling, federal funding agencies and academic organizations might desire that wider economic impact assessments be carried out to justify sustaining or even increasing R&D expenditures in the areas of materials modelling.

Economic accounting-based methods that are often used for impacts assessments, such as input-output analysis, social accounting matrices, or any model that operates on a static economic structure, are not ideal for modelling the types of supply side changes that will result from the introduction and wide-spread use of materials modelling software and outputs. These models operate by specifying demand shocks and determining the impacts of increases in demand for existing commodities, services, and production processes. When the commodities or services demanded are new or the production process associated with the commodities or services is sufficiently different than some representation of an average existing industry, these models will fail to accurately estimate economic impacts. However, the availability of standardized software such as IMPLAN©[1] for analyses in the United States make these types of analyses ubiquitous in both private and public assessment of materials modelling and its applications.

When modelling the introduction of new technologies or a new way of doing business for an existing industry, dynamic simulation models, such as interindustry econometric models or computable general equilibrium models, are more appropriate and adaptable. However, these models do not exist in a standardized form. Appropriate modelling will be scenario specific and necessitate someone with a high level of both problem domain knowledge and modelling domain knowledge.

2. Assessing the impact of materials modelling research

Materials modelling attracted substantial amounts of grant funding over the last 20-30 years. For example, in the European Commission's 7th Framework Programme (2007-2013) about 100 projects involving materials modelling [2] were funded within the the Industrial Technologies programme.

Materials modelling is closely linked to academic research and hence understanding and determining the wide range of research impacts is important to gain a full perspective. In order to assess the impact of research, the four commonly used approaches [3] cover bibliometrics, case studies, peer review, and economic analysis. A previous report [4] reviewed the evidence across these and other indicators including:

- Publications and patents
- Growth of populations of beneficiaries of modelling such as users of models and end-users of modelling results
- Success stories
- Acceptance of molecular modelling by peers in industry
- Macro-economic impact models

Some pertinent findings from the economic impact report [4] are summarised below.

Bibliometrics

A strong, above average, rise in the number of publications in materials modelling and an above average impact factor have been demonstrated by a number of studies (see [4] and references

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therein). Evidence included detailed bibliometric analysis in the field of simulation-based engineering and a study of publications involving electronic density functional theory. Also, patents based on one of the key models (Electronic Density Functional Theory) rose much more strongly than average in the last decade.

Human Capital

A strong rise in the number of researchers involved in modelling was found (see [4] and references therein). In particular, there are ever expanding circles of influence of modelling from the original authors to the beneficiaries of modelling. Whereas in the 1980s the authors of modelling were also the users, the group of users is now much bigger and in recent years an even larger group of 'consumers' of modelling results has emerged.

Macro-economic indicators

The contribution of discrete materials modelling to chemistry research and high performance computing was quantified [4]. Since other studies quantified the contribution of these activities to GDP, a tentative link between materials modelling activity and macro-economic data could be made.

Case studies from the UK Research Excellence Framework

In the United Kingdom (UK), the Research Excellence Framework (REF) was established as the new system for assessing the quality of research in UK higher education institutions [5] and the first REF exercise was conducted in 2014. The research of 154 UK universities was assessed, and 1,911 submissions were received detailing 6,975 impact case studies of UK academic research. Impact assessment was carried out based on the criteria of 'reach' and 'significance', see [6] for a discussion on impact assessment.

Here, we consider the REF submissions as a useful source of case examples. A search for terms such as materials modelling and computational chemistry yields the following 15 directly relevant case studies (see Appendix: UK REF exercise), with a much larger number involving some sort of modelling in relation to materials. Six of the cases include different software packages (CASTEP [7], MOLPRO [8], TOPAS [9] and DL_MESO [10]) with significant industrial impact (in case of CASTEP more than $30M software sales). Other impacts reported included improved product innovation and design, spin-off companies, enabling breakthroughs in industrial R&D projects via collaboration, improved product quality and reliability, reducing environmental impact due to lightweight recyclable materials, reduced energy processes, etc.

3. Materials modelling for industry

The drivers of impact assessment have been expressed as the four 'A's: advocacy, accountability, analysis, and allocation [3]. These are not only important in the public realm of research funding and for research impacts more widely, but equally in economic impact assessment and the justification of resources in R&D in the private sector. Here we review some evidence from previous studies of the materials modelling and ICME sectors, recent patents by the Boeing Company, as well as a study considering how modelling as an organisational function in industry can improve its impact.

R&D process improvements

An earlier study by market intelligence company IDC [11] on the ROI of molecular modelling in the materials industry was recently re-analysed in detail [4], in particular considering lower costs of software and hardware. The ROI on investment in molecular modelling of approximately a factor of 7 was found to be reasonable, resulting from a combination of more efficient experimentation, broader exploration, deeper understanding, saving a product development project, and/or accelerated product development as well as in some cases improved safety testing and hazard avoidance.

Integration with engineering

As was already outlined in our previous Economic Impact Report [4] there is strong evidence that the integration of materials modelling with engineering workflows (so-called Integrated Computational Materials Engineering) has been carried through successfully with a large return on investment.

ICME goes beyond materials modelling and involves the integration of personnel, models, computational tools, experiments, tests, analyses, design, and manufacturing processes across the entire product development program [12]. The Minerals, Metals, & Materials Society published a study [13] on Implementing ICME in the Aerospace, Automotive, and Maritime Industries, which includes some pertinent considerations regarding economic impacts.

Due to the comprehensive remit and the fact that ICME is a relatively new discipline there are still relatively few documented case studies. ICME has just begun to demonstrate its potential to accelerate product development processes, to yield improved ROIs, and to improve the quality of life for consumers. The prominent industrial demonstrations of the potential of ICME are (see [13] and references therein):

- A project led by Ford Motor Company is reported to have yielded a 7:1 ROI and a corresponding 15%–25% reduction in development time and led to a lighter engine design. See also the outline of this study in our previous report [4].
- GE Aviation utilised an ICME approach to achieve a reduction of the rhenium (a rare and expensive element) in superalloys for aircraft engine turbine airfoil components. The ICME approach taken resulted in the introduction of a new alloy in two years rather than the typical six years historically required for such a new alloy.
- QuesTek Innovations led a project that resulted in the development of the corrosion-resistant Ferrium S53 advanced high-strength steel alloy for landing gear and other applications. The ICME approach led to significant reductions in alloy development time and an estimated development cost savings of nearly $50M.

Further successful ICME case studies are included in publications such as the National Research Council ICME Study [14], Integrative Computational Materials Engineering, edited by Georg Schmitz and Ulrich Prahl [12], and Integrated Computational Materials Engineering (ICME) for Metals by Mark Horstemeyer [15].

Further evidence of the value derived from materials modelling and its integration into engineering can be gleaned from three recent patents by the Boeing Company. Boeing has been very active in the materials modelling field down to the chemistry level for some time [16,17]. Rather than relying on the traditional supply chain dynamics, Boeing got involved in chemistry based research *in-silico*, taking a pro-active role in shaping its own future across all disciplines.

The three patents [18,19,20] demonstrate the significance of the corner-stones of exploitation of materials modelling at the industrial level, which are also highlighted by the ICME studies [13,14] and in the European Materials Modelling Council (EMMC) roadmap [21], i.e. (a) materials modelling has been developed to a point that it can make an impact on real industrial problems, (b) multi-scale modelling workflows are key to realising impact, (c) it is important for business efficiency and effectiveness to integrate information gained down to the chemistry level into wider information management and business decision support systems.

Testimony to (a) is "Fiber-reinforced resin composites and methods of making the same" [18]. It deals with the efficiency of load transfer between the fibre and the surrounding matrix at the micro-scale level, which may directly affect the overall mechanical performance of the composite at the continuum level. "The region of the matrix that may be substantially affected by the presence of fibres, sometimes referred to as the "interphase" region, is the interfacial area of the matrix directly surrounding the fibre. In composites, this interphase region may experience high shear strain due to the mismatch in elastic stiffness between the fibers and the surrounding matrix. Widely-used conventional bulk resins may not provide desirable distortional capabilities." The patent claims superior performance of resins developed with the help of atomistic materials modelling. This performance improvement could translate into substantial efficiency in load bearing and associated lower weight of the aircraft frame.

Testimony to (b) is "Multi-scale modeling of composite structures" [19]. The patent basically claims that there is a controlled, deterministic relationship between composite performance and materials/chemical structure at various levels, as calculated by modelling: "A method, apparatus, and computer program product are present for creating a composite structure. A number of characteristics for a number of components for the composite structure is obtained from a simulation of the composite structure using a model of the composite structure. A number of changes in the number of characteristics needed to meet a desired level of performance for the number of characteristics is ascertained. A number of attributes for a number of composite materials used to form the number of components corresponding to the number of characteristics having the number of changes is identified. The number of attributes for the number of composite materials for the number of characteristics having the number of changes based on the desired level of performance is changed."

Testimony to (c) is "Product Chemical Profile System" [20]. The abstract describes a system that is able to pull together and query all levels of information about a product down to the chemistry level: "A computer-implemented system and method for obtaining product related information obtained from a plurality of different sources that is transformed into processed product data with a plurality of levels. Callouts and contexts are identified and a product-to-chemical continuum is generated by creating callout-context pathway segments between the plurality of levels of the processed product data based on the callouts and contexts identified and a transformed query request is generated used to traverse the product-to-chemical continuum through the callout-context pathway segments that span the plurality of levels. The product information that matches the set of context search parameters is extracted from the product-to-chemical continuum. The callout context pathway segments reduce processing resources and time needed to obtain the product information."

These patents are a clear recognition of the relevance and importance materials modelling and an integrated approach to engineering at a world-leading company.

Making a business case

Convincing stakeholders to adopt ICME methods as a way to discover, develop, and deploy advanced materials cheaper and faster can be a challenge. The modelling software, supporting databases, and qualified personnel are significant investments to begin an ICME-accelerated product development programme, and are often viewed as a substantial business risk from the perspective of management. Typically, stakeholders rely on numerous relevant case studies to develop a plan with a sound business structure and fiscal strategy to ensure they achieve their expected ROI, but these are still in limited supply for ICME.

Examples of successful implementation are valuable in making the case for implementing materials modelling and, more widely, ICME. However, the "Implementing ICME" study [13] emphasises the critical importance of a sound business case that demonstrates the value and ROI for stakeholders (e.g., materials suppliers, manufacturers, and designers). In fact, the first pervasive issue identified in the study is to "Create a business case for ICME". Issues that companies new to ICME will inevitably encounter are identified and tactics to construct a business case are outlined.

To develop a strong economic case requires a sound quantitative analysis of risks, costs (capital and time), and benefits associated with technology development and implementation.

Typical benefit categories identified by the ICME study [13] include:

- Decreased testing requirements
- Reduced risk, time, and iterations for the materials and process development
- Elimination or reduction of costly traditional product iterations
- Guide patent development and even reverse-engineer product patents from existing products

In line with its focus on engineering in aerospace, automotive, and maritime industries, the more specific potential savings are related to materials testing, certification, and design allowables:

- Testing costs and duration can be quantified in a number of areas. For example, certification costs associated with each product or part are ongoing, yet the volume of certification tests required could diminish significantly because of model simulations.
- Validation tests for materials suppliers will decrease as models become more representative of real-world conditions.
- Design allowables: as computational methods and databases are becoming more advanced regarding predictive methods, fewer tests are required to establish the confidence needed to develop new design allowables specifications.
- Passing the quality requirements of the Materials Review Board is time consuming and costly, particularly if temperature, chemistry, or processing costs do not meet certain conditions, when this may otherwise have been avoided by computational methods.

- Developing statistical or neural net models from relevant materials databases as part of the development of new materials may be easier to achieve with the advancement of robust, physics-based predictive tools.

The study points out the importance of integrating the materials modelling based options into an overall systems approach for the economic case, including materials characteristics, manufacturing process, product design, and business criteria. Such an integrated Business Decision Support approach is also called for in the EMMC Roadmap [21].

Typical cost categories identified and issues to consider are:

- Software licenses and high performance computing resources often require significant funding, particularly in early stages of development. It may take a long time (whole product development cycle) to realise savings overall.
- An IT infrastructure for the generation, capture, and transmission of data, as well as the generation of relevant physics-and experience-based modelling tools.

Workforce needs are also addressed in the study, in particular in relation to the lack of trained staff rather than as a cost factor.

Performance metrics for a modelling function in R&D

It is useful to consider the experience of modelling functions in the pharmaceuticals industry. Modelling and simulation in life science and its application in the pharmaceuticals industry has always been ahead of the materials science area by about a decade. The first computer-aided drug discovery (CADD) company (MDL, which eventually found its way into what is now Biovia) was founded in 1978, followed by Tripos in 1979, whereas the first start-up with a focus on materials design was Cambridge Molecular Design in 1989 (which in fact also ended up in Biovia).

Since CADD is in such wide-spread use in the pharmaceutical industry, what can be learned from experiences there regarding impact and its metrics? During the 'boom years' of the pharmaceuticals industry, spending on R&D increased dramatically, and very substantial investments were made in CADD. However, the sector has come under significant pressure in recent years, undergoing major organisational changes and cost-cutting. Hence, all areas of the R&D process have come under increased scrutiny, and the importance of demonstrating impact of a CADD has become much stronger.

An interesting exercise in defining metrics and measuring impact was by scientists from Bristol-Myers Squibb [22]. They point out the reservations of CADD scientists to metrics: metrics being irrelevant to the creative function performed and might be misused to direct focus on mundane tasks of little scientific interest or importance and eventually to fire them. Hence, the first step is to establish knowledge about and trust in metrics. Key to that and to successful metrics was a clear mission for the R&D function, which includes a What, When and How. In the case example, the mission was stated as follows:

"To guide the identification, selection, and optimization of drug candidates and targets through the application and development of molecular modelling, data analysis, and computational chemistry techniques."

Based on the mission statement, three levels of impact were defined:

- Level 1: CADD provided data from their modelling to other functions in the organisation.
- Level 2: The data triggered a response action that led to consistent results, for example characterised and/or synthesized a compound that showed the effects indicated by the model.
- Level 3: Project leader agrees in writing that CADD made an essential contribution to the project progress. (Would not have progressed without it).

The impact levels, including data, analysis, scientific decision support, and programme impact are also shown graphically in Figure 1, which is adapted from [3] for the case of materials modelling. At Level 1, data are provided to an R&D programme, followed by analysis. At Level 2, the information provided by modelling has an impact on individual steps in an R&D process. This in itself typically leads to cost and time saving. At Level 3, modelling has led to improvements in the overall outcome such as a new/improved material, process or component.

Similar mission statements and Key Performance Indicators (KPIs) would be highly recommended for the materials modelling function in industry. Of course they will vary by sector and by where the company is in the supply chain, but the principles remain the same.

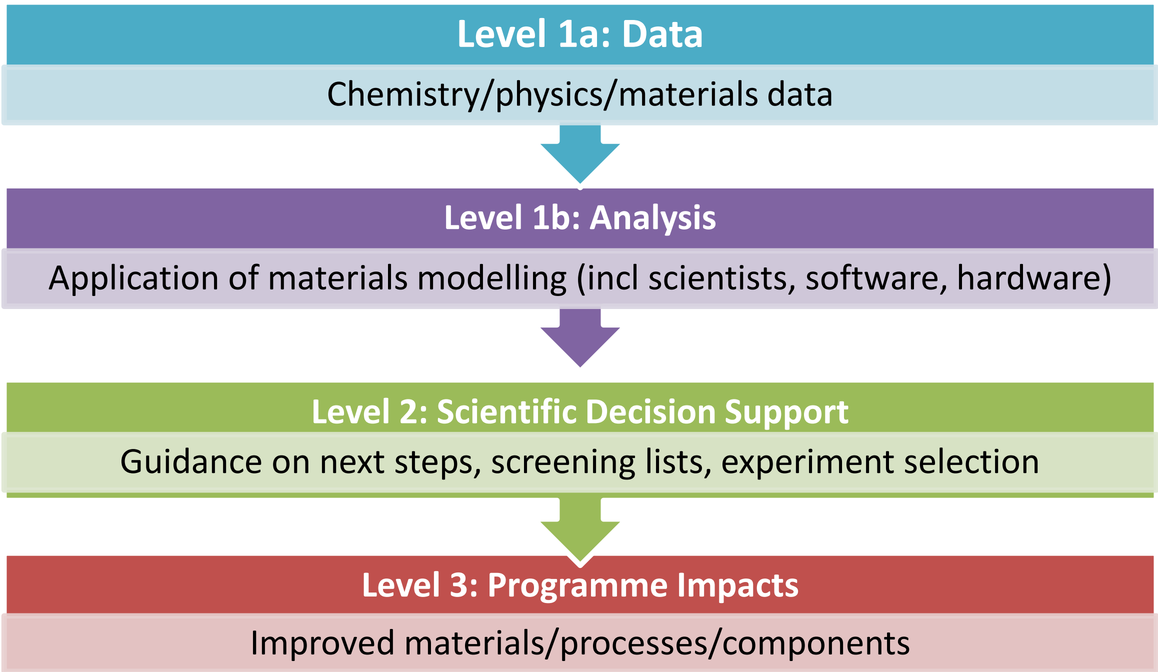


Figure 1: Levels of Impact as identified for CADD and adapted for Materials Modelling.

In the case example reported by Bristol-Myers Squibb, the impact metrics exercise led the organisation to use its resources more efficiently and effectively. The number of projects where no contributions could be made fell while there was a strong rise in projects with Level 2 and Level 3 impact over a four year period.

This increased focus meant:

- Avoiding “nice to have” modelling requests
- Constantly keeping an eye on whether projects have an impact
- Thinking strategically about resources
- **Focus discussions regarding software around problems, not technologies**
- Actively avoid a “shots on goal” approach to staffing projects. Metrics show that deeply involved, focused, support is more impactful than in-and-out drive-by CADD work. It was found that short in-and-out projects tended to be a wasted effort, that people with sufficient depth of knowledge are needed to make sense of the data. In fact, this point is also emphasised strongly in the EMMC Roadmap for Materials Modelling, in particular highlighting the need for so-called Translators. See [21] for further details.
- Focus innovation projects on improving observed issues

4. Economic impact survey

An online survey was conducted in spring/summer 2015 with the support of the EMMC and the European Commission Directorate-General for Research & Innovation, Directorate D: Key Enabling Technologies. The survey is available online and as a separate pdf document [23].

The aims of the study were:

- To compile success stories and case examples involving materials modelling in academia and industry
- To improve the understanding of the benefits of using materials modelling
- To help quantify the impact of materials modelling
- To support decisions by public bodies and private organisations

The survey elicited information about R&D projects that significantly involved materials modelling and that led to an innovation, a product improvement, or a new product. Participants were asked for some qualitative information about the project, the innovation and benefits of materials modelling, as well as some quantitative information about the ROI of the project as a whole.

The following qualitative impact indicators were probed:

- Description of the benefits in terms of the R&D process, the innovation, and the impact created
- Identification of the key task that modelling was used for, with choice between materials property data, insights, or an ‘other’ description given by the respondent
- Identification by the respondent of one of the key benefits associated with materials modelling by the 2004 IDC study
    - More efficient and targeted experimentation
    - Avoiding potentially hazardous experimentation
    - Broader exploration
    - Deeper understanding
- Types of impact achieved
    - Innovation accomplished
    - Revenue increased
    - Costs saved

- Jobs created

As quantitative indicators of ROI, the following economic impact variables were requested:

- Overall revenue generated, i.e. the company's total revenue generated that can be directly related to the final product incorporating the material that resulted from the modelling process. The main point here was to keep things simple and just consider the revenue of the final product as a whole rather than associate a particular portion to materials modelling. The same approach was used by IDC in a pilot study on the ROI of investing in High Performance Computing (HPC) [24].
- Cost saved. Modelling is often used to direct experimentation and avoid dead-ends with clear cost savings that might be relatively straight forward to identify. Also, there are a number of examples where modelling has led to more efficient manufacturing routes or cheaper materials, again with clear cost savings.
- Number of jobs created
- Investment made in modelling hardware, software, and staff. Regardless of impact details, companies don't make investment decisions lightly. Hence, the fact that significant investments are made in industry can serve as an impact indicator, especially if traced over time.

The target group of the survey were industrial end users of modelling. Invitations were sent to about 150 manufacturing organisations (the majority of which are located in Europe). In addition, a few research organisations and software owners involved in relevant European projects were also invited to take part.

Responding organisations

A total of 34 responses from manufacturing organisations were obtained representing a response rate of about 23%. Five of the responses were from materials manufacturing companies that have been involved in projects where modelling was carried out but that are not involved in modelling now or do not carry out materials modelling within the organisations. The latter is indicative of a significant segment of typically mid-sized manufacturing companies that have an interest but are not ready so far to take the technology in house. This then left 29 responses for further analysis.

The manufacturing companies that responded include a range of Small and Medium Enterprises (SMEs) and global players as indicated by the revenue range of the organisations shown in Figure 2. A wide range of industry sectors are represented, including automotive, chemicals, consumer goods, electronics, and structural materials.

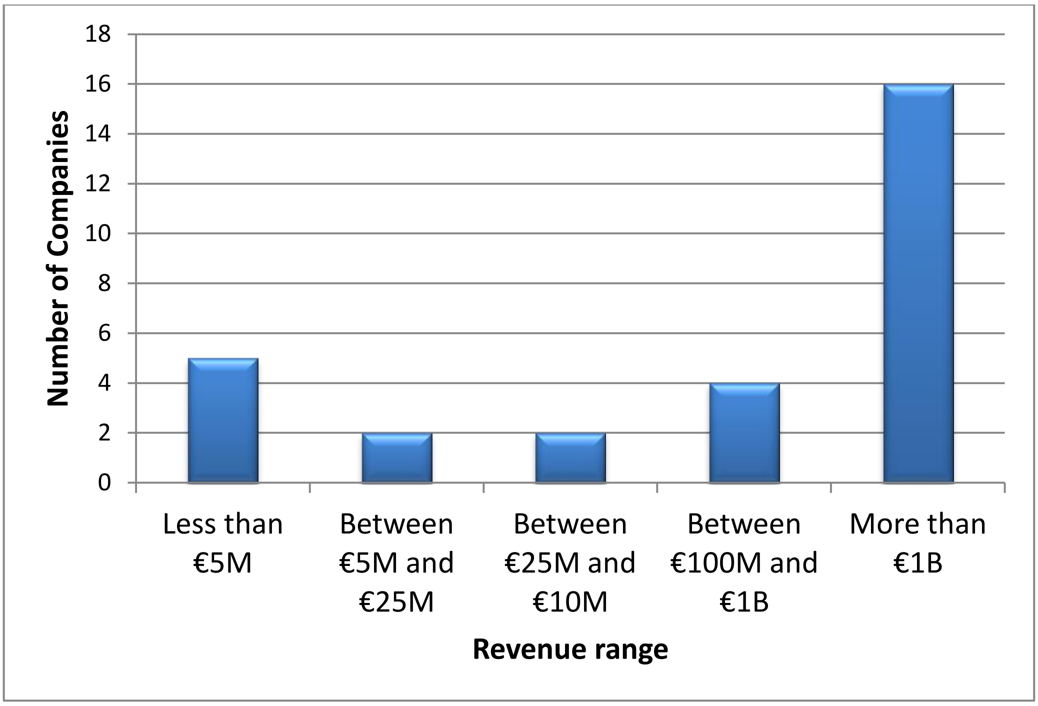


Figure 2: Revenue ranges of responding organisations

Types of materials modelling used

Although atomistic modelling is the most widely used type of materials modelling across survey respondents, responses indicate that all types of modelling were covered well in this survey, as shown by the chart in Figure 3.

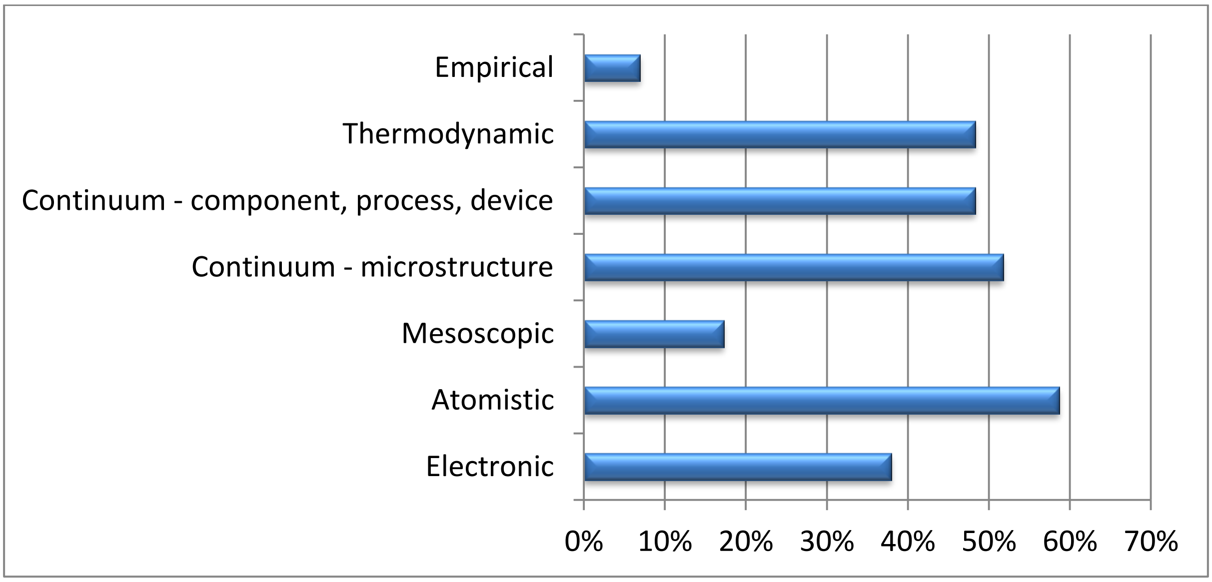


Figure 3: Types of Materials Modelling Used: Since respondents were asked to select all that apply, the total adds to more than 100%.

Discrete modelling (i.e. electronic, atomistic or mesoscopic) was used in 62 % of the organisations; 83% used discrete and/or microstructural modelling and 41% used a combination of discrete and continuum or thermodynamics models.

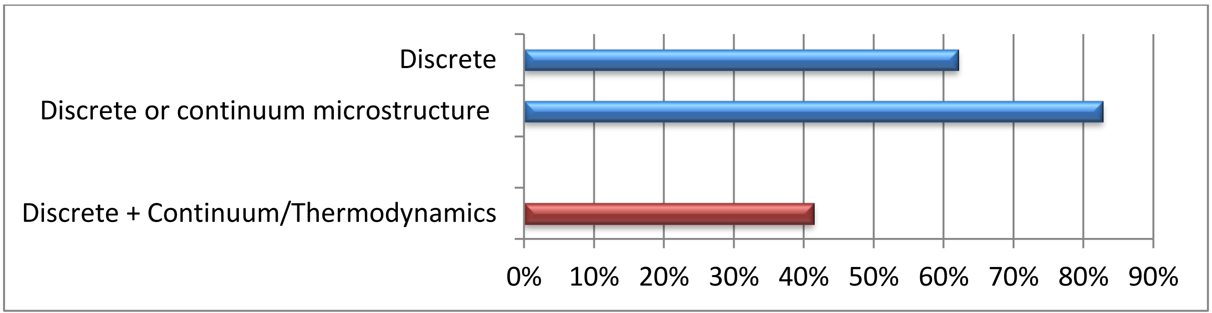


Figure 4: Types of Materials Modelling Used

Scales of modelling applications

The wide usage of discrete and microstructural modelling is also reflected in the length scales that were probed (see Figure 5), with most projects involving nanoscale phenomena. Five organisations investigated phenomena across all scales and only three of the 29 responses involved purely macroscale phenomena.

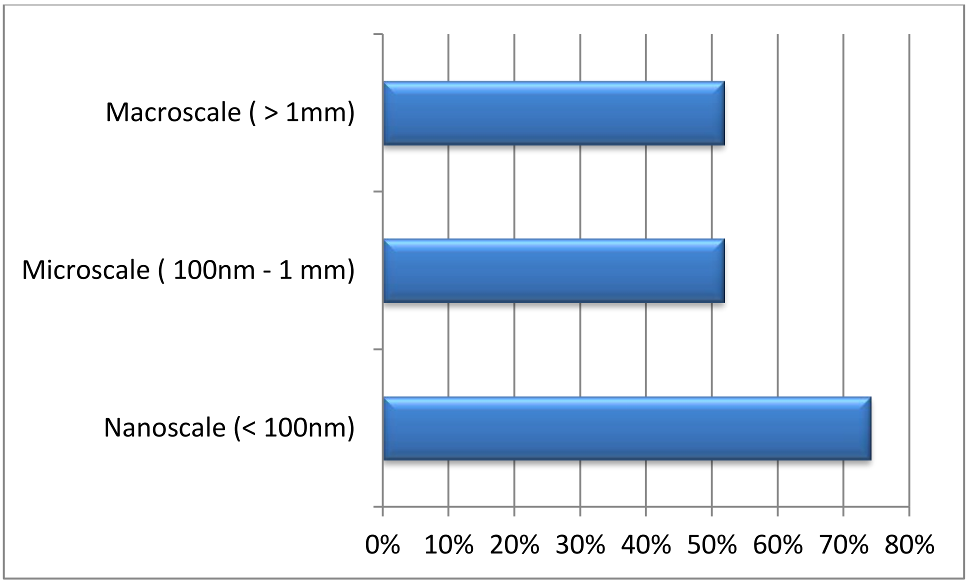


Figure 5: Scales investigated by materials modelling.

Project descriptions

Although most respondents only permitted general and average information to be shared for reasons of confidentiality, the following excerpts of the project descriptions (which in some cases had to be shortened and suitably anonymised to retain confidentiality) provide some insights into the range of projects and applications.

Applications

- Synthesis of new materials
- Catalysis including in fuel cells
- Coatings; nanostructured coatings and thin films deposition on cutting tools
- Study of multi-layered surface systems by developing robust multiscale materials modelling
- Magnetic materials; reduce the usage of rare earths
- Structured materials applied to renewable energies
- Gas sensing
- Functional materials: ceramic pigments
- Electronic and phononic transport in graphene for energy accumulation devices
- Compounding and injection moulding of polymer matrix nanocomposites for lightweight applications
- Composites; nanocomposites; mechanical performance of laminates and industrial components; process, structural behaviour, and multi-functionality (conductivity, environmental protection, damping, ice protection, lightning protection)
- Decorative engravings, marking and microscopic mechanical improvements
- Adhesive properties of industrial polymers
- Polymeric materials: study of polymer degradation route; adhesive properties of industrial polymers
- Formulations: performance of a formulation depending on the solvent used, to select the optimal solvent
- Metallic materials (nanostructured coatings and thin films deposition on cutting tools)
- Alloys: Melting/solidification; Crack formation and propagation in cast light alloys
- Steel: forming; stretch bending limits; effect of defects on fatigue strength
- Process simulations of multi stage metal forming, heat treatments and multi-physics processes in a production chain
- Powder metallurgy (compaction and ejection; sintering; porous metal plasticity during hot forming of sintered parts)
- Hydrogen diffusion in metals
- Additive manufacturing
- Aero engine components

Qualitative impact indicators

The descriptions or projects and innovation achievements provided a rich source of information about the wide range of benefits and impacts achieved by using materials modelling.

A broad overview was obtained by a couple of multiple choice questions. The first question regards the two main 'modes' of materials modelling [25], namely the discovery mode, which is about insights and understanding and secondly data-driven simulations that aim to achieve accurate (and/or controlled error) property determination (see Figure 6).

The second question pertains to the typical R&D process improvements that were identified in an earlier impact study of molecular modelling in the materials sector by IDC [11].

Mode of materials modelling

Discovery mode (gaining insights) and data-driven simulations (determining properties) have roughly equal weight and were both applied in about 70% of cases.

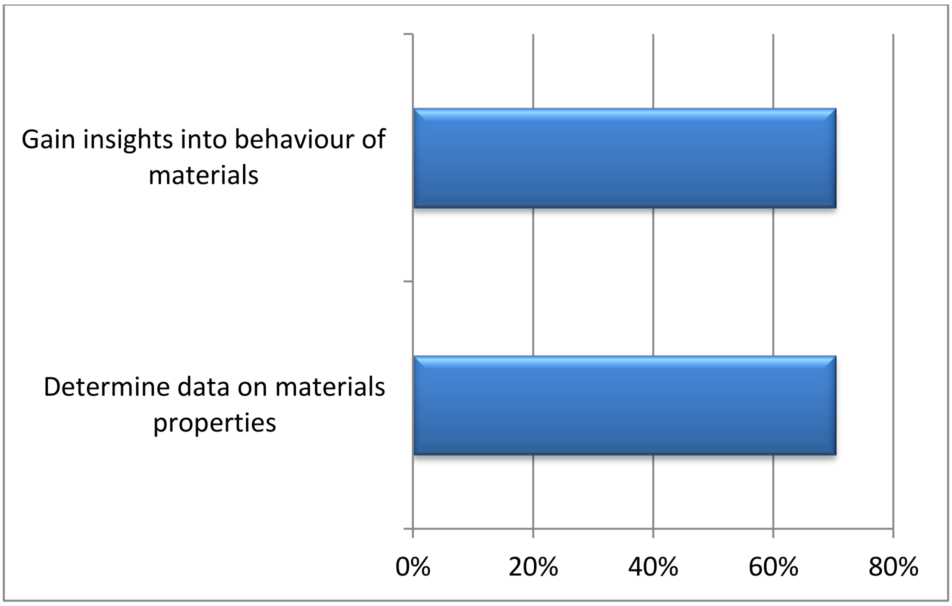


Figure 6: Modes of Materials Modelling Employed

R&D process improvements

The typical R&D process improvement benefits agree with those already identified in the IDC study, as shown in Figure 7 (see also Section 3 on R&D process improvements).

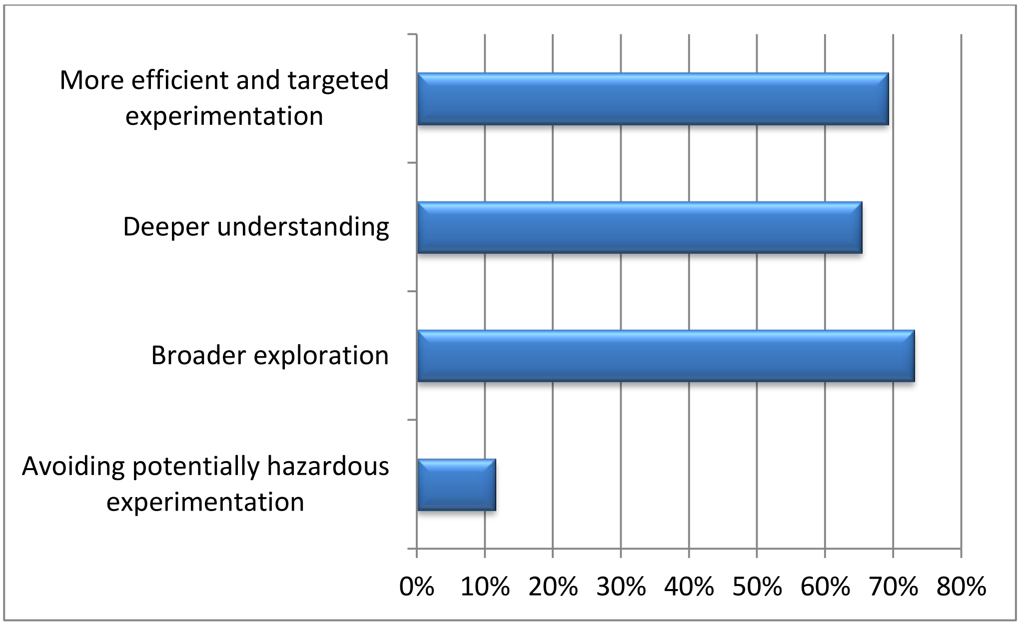


Figure 7: R&D Process Improvements

Key Performance Indicators of R&D and business benefits

The responses demonstrate that there are multiple avenues through which materials modelling creates impact. It supports and improves the R&D process in various ways that contribute to smarter R&D, an increased probability of innovation success, saving cost and time, improved flow from R&D to production and marketing and an increased certainty in making business decisions. The following KPIs were obtained from the responses, each illuminated with examples taken from the survey responses:

More efficient and targeted experimentation

- Pre-selection of chemicals/materials instead of experimental testing of a larger set
- Reduce the screening by experiments (cost, time)
- An exploratory tool to minimize lab tests
- A set of solvents was proposed for further experimental screening. Doing a pre-selection of solvents, selecting ca. 10 out of a set of >1000, which takes only about one day, saves a lot of time compared to experimental testing of a larger set, based on intuition.
- Determine whether a target performance is easy to reach, just doable, or impossible
- Evaluation of process deviations without the necessity of destructive testing

Source of property data

- Prediction of the basic physical properties and thermodynamic phase equilibria of complex organic molecules
- Determine data on materials properties
- Completely substitute experimental measurements
- Materials modelling was able to explain differences in material performance, whereas traditional standard test method could not distinguish the materials.

Broader and more efficient exploration

- Routes to new polymeric materials by prediction of chemical kinetics and thermodynamics successfully used for technology identification (i.e. new molecule development)
- Modelling helps to determine whether a target performance is easy to reach, just doable, or impossible.
- Exploring a completely new field

R&D strategy development

- Design of the strategy for obtaining the new materials (i.e. at the start of a programme rather than guidance during a programme)

Deeper understanding

- Gain insights into behaviour of materials and underlying physics/chemistry
- Understanding of physical process, property prediction and a deeper understanding of specific processes; contributes to faster developments of materials
- Understanding mechanism of action for how our materials perform
- Validation of theories (concerning hydrogen diffusion e. g. influence of grain boundaries, the role of trapping sites)
- Provide understanding of physical phenomena (mainly thermomechanical) of new and existing materials, currently and to be used in our future projects

- Description of forming limits of steel sheet
- Fundamental understanding of phenomena aiding design from material synthesis to device design
- Validation of synthesis routes

Trouble shooting

- Trouble-shooting and avoiding dead ends (also due to improved insights), for example trouble-shooting issues relating to product stability

Performance optimisation

- Enabling optimisation of existing products and processes. Trade-offs are very hard to determine without models that describe all relevant phenomena. Optimisation includes the ability to set engineering design limits for structural components, which saves weight and cost. For example, a cheaper steel grade or a thinner wall thickness might be sufficient, but a detailed and accurate model is required.
- Optimized formulation to disperse a specific ingredient, and the development of a generally applicable method to quickly select a set of potentially high-performing solvents
- Device/nanostructure analysis and optimization at all the relevant length scales
- Optimisation of the material composition and structure in order to have the best output performance on the device level

IP protection for innovations

- Materials modelling is used quite widely in underpinning intellectual property (IP), supporting patents and in cases staking a wider claim.

Value chain benefits

- Build up a relation between product accuracy, intrinsic properties of the material used and the production process of the materials supplier
- Validation of supplier information on materials datasheets

Improving collaboration and communication between R&D and production

- Modelling as a bridge between process engineers at the production site and researchers in the R&D centre

Upscaling and market introduction benefits

- Providing the level of detail in know-how about the product that lowers the technical risks of upscaling and market introduction
- Providing the missing link between small scale material testing and large scale application results
- Modelling and simulation allows testing and verifying new manufacturing strategies although they were not physically available at that time.
- Understanding material behaviour in application (forming, crash, ...) via modelling
- Compare material properties and link that to performance in real applications
- Detailed process understanding resulting from modelling supports a faster and more assured market introduction.
- Linking the small scale material testing with large scale application results

Marketing and competitive benefits

- As a result of materials modelling the benefits of our materials compared to competitive materials could be demonstrated to customers.
- A pedagogic and marketing tool to explain the technology through visualisation
- Modelling of material behaviour in its downstream application (e.g. forming, crash ...)

Quantitative impact factors

The impact of materials modelling on a number of outcome measures was surveyed in order to arrive at a more quantitative assessment. The main categories were innovation, costs savings, revenue increase, and job creation. Figure 8 shows the percentage of organisations that identified these types of impact. Not all respondents were able to contribute quantitative information on the above impact factors, but following is an analysis of the replies received.

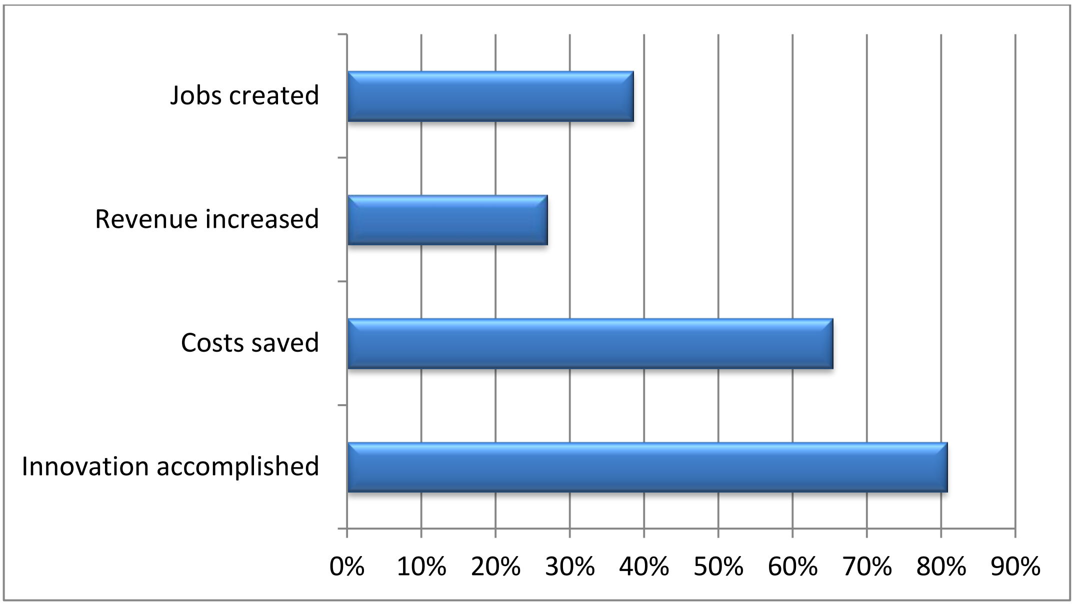


Figure 8: Quantitative Impact Factors Reported

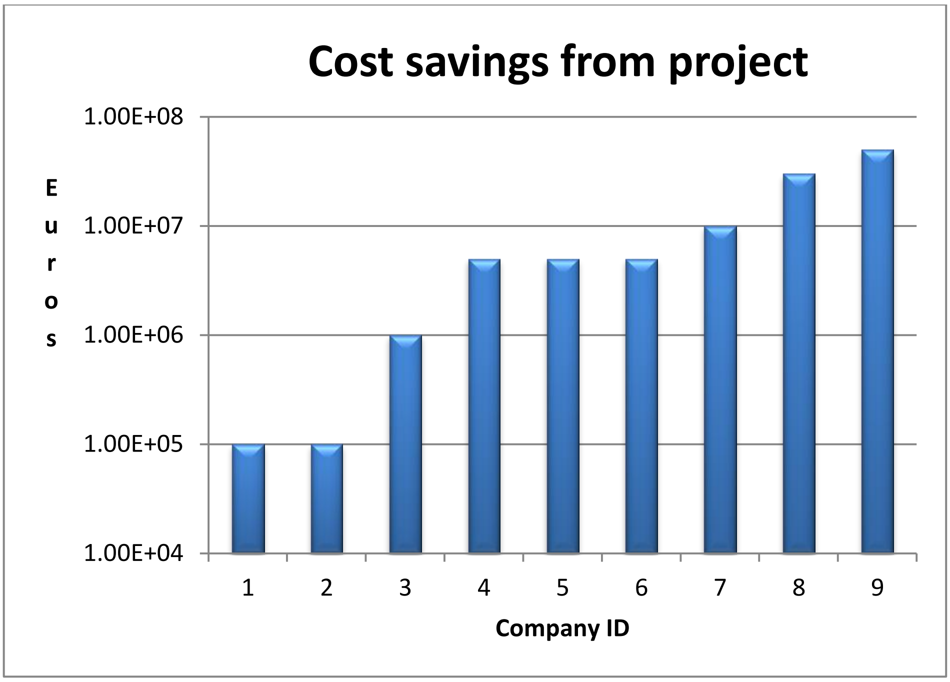
Innovation

Innovation drives value and based on the benefits described above it is expected that modelling has a strong impact. Indeed, 81% of respondents reported Innovation as a result of materials modelling.

Cost saving

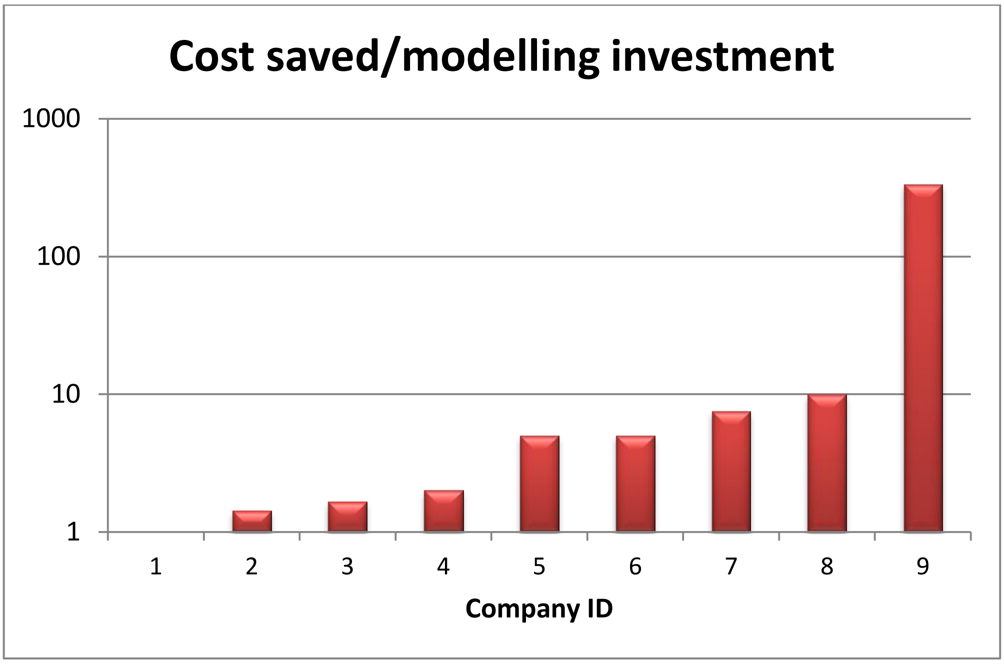
Modelling is widely used to increase R&D efficiency, and it helps to reduce product costs by identifying alternative, more cost effective materials and processes. For example, one project resulted in cutting development time from 10 to 1.5 years, saving millions of euros because of the understanding of the material and saving of experiments.

Nearly two thirds of projects reported cost savings. Absolute cost savings due to the materials modelling project ranged from €100K to €50M (see Figure 9) with an average of €12M and a median of €5M. Costs saved as a multiple of the investment in materials modelling ranged from 1 to 300 (see Figure 10), with an average of 41 and a median of 5.



Note: The ID given to a particular company varies across Figures.

Figure 9: Cost savings resulting from the materials modelling projects for the nine organisations that reported these figures.

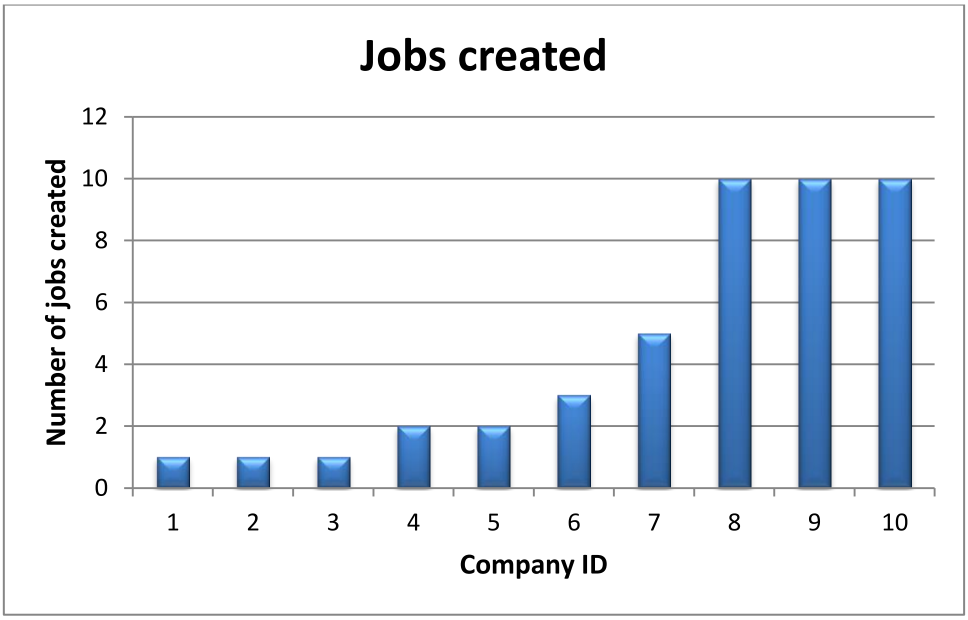


Note: The ID given to a particular company varies across Figures.

Figure 10: Costs Saved/Modelling Investment.

Jobs created and investment in staff

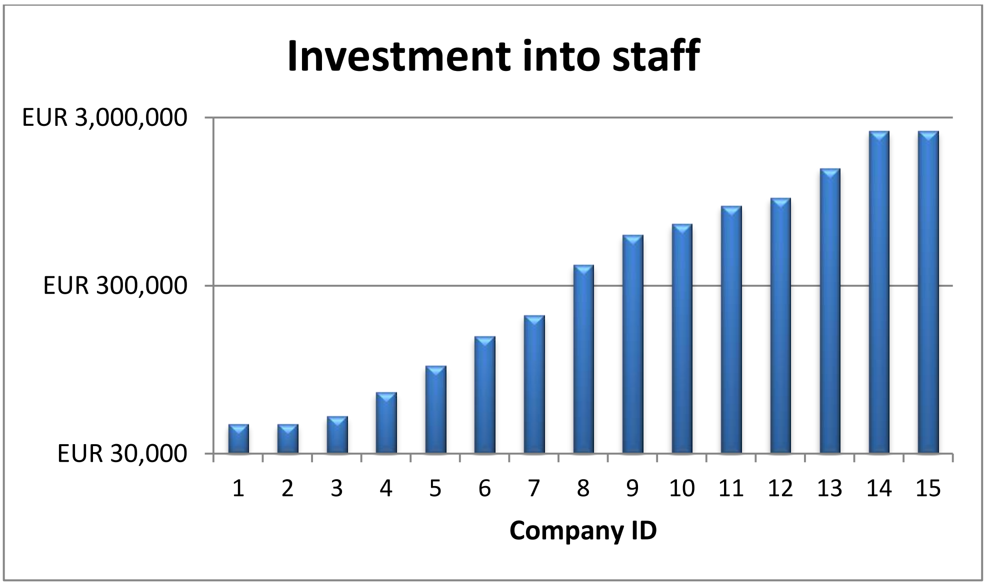
As shown in Figure 11, in about 35% of cases new jobs were created for the modelling projects, with the number reaching up to 10.



Note: The ID given to a particular company varies across Figures.

Figure 11: Jobs Created.

A wider range of responses were obtained for investment into staff carrying out the materials modelling projects (Figure 12), ranging from €45,000 to € 2.5M, with an average above €700K and a median of €400K.



Note: The ID given to a particular company varies across Figures.

Figure 12: Investments in Materials Modelling Staff.

Investment in materials modelling projects

While ROI is a widely accepted indicator of impact, it can be argued that industry does not make any investment without good business reasons. Materials modelling is often pursued as a means of providing better insight and understanding, which can be hard to quantify directly. Hence, it seems reasonable to consider the direct investment made by industry in materials modelling as an indicator of impact.

Nineteen organisations provided information about the investment in the materials modelling projects (see Figure 13), most of them also broken down into staff, software, and hardware costs. In addition, total costs of the R&D project, i.e. including all other R&D activities carried out in the project, were obtained. The average investment into materials modelling was €940K and the median €475K.

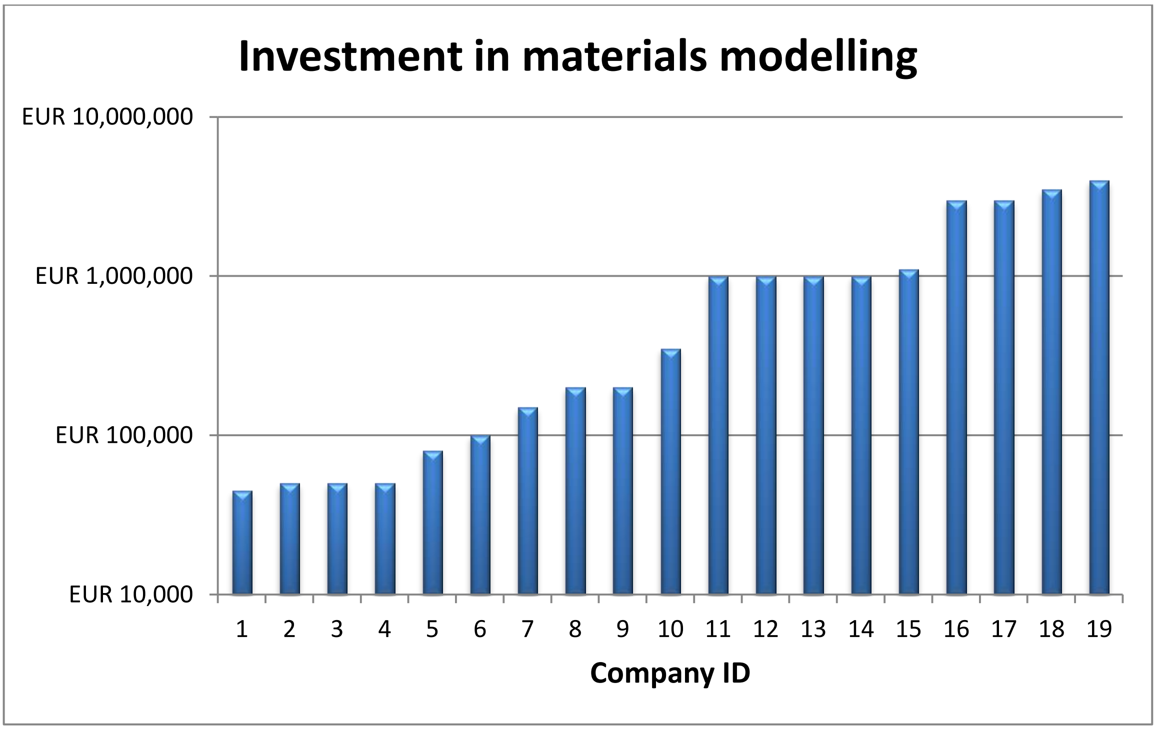


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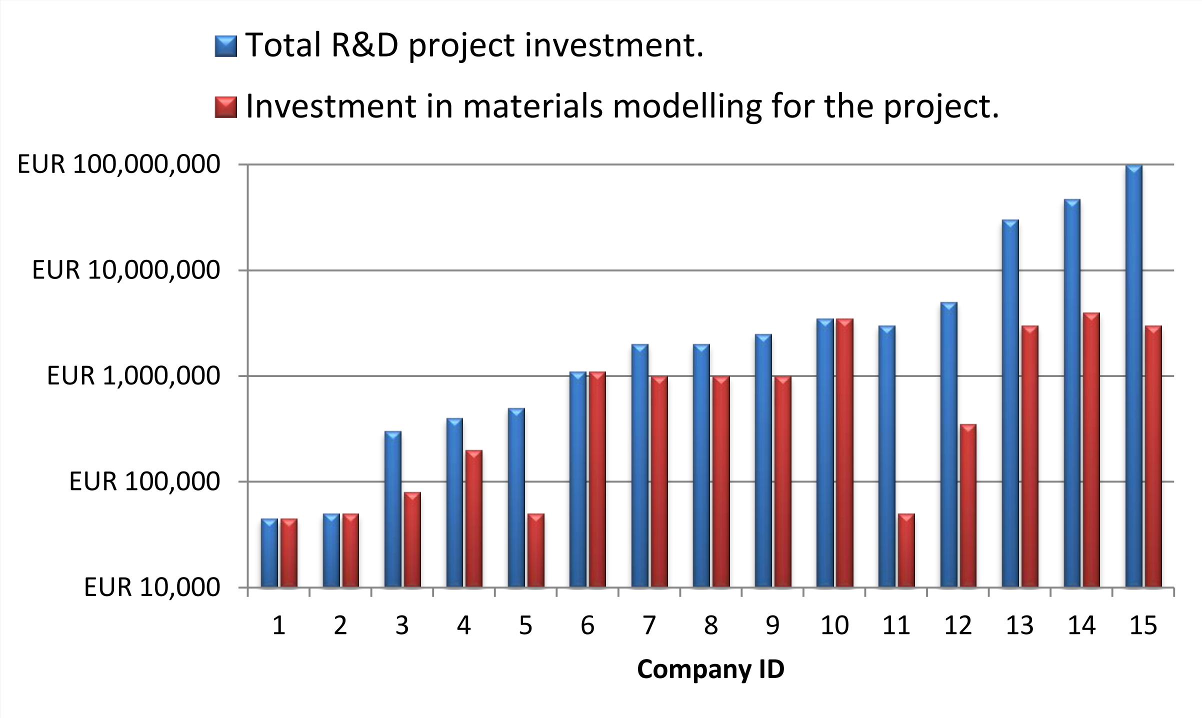
Figure 13: Total investment in the materials modelling projects described by nineteen companies.

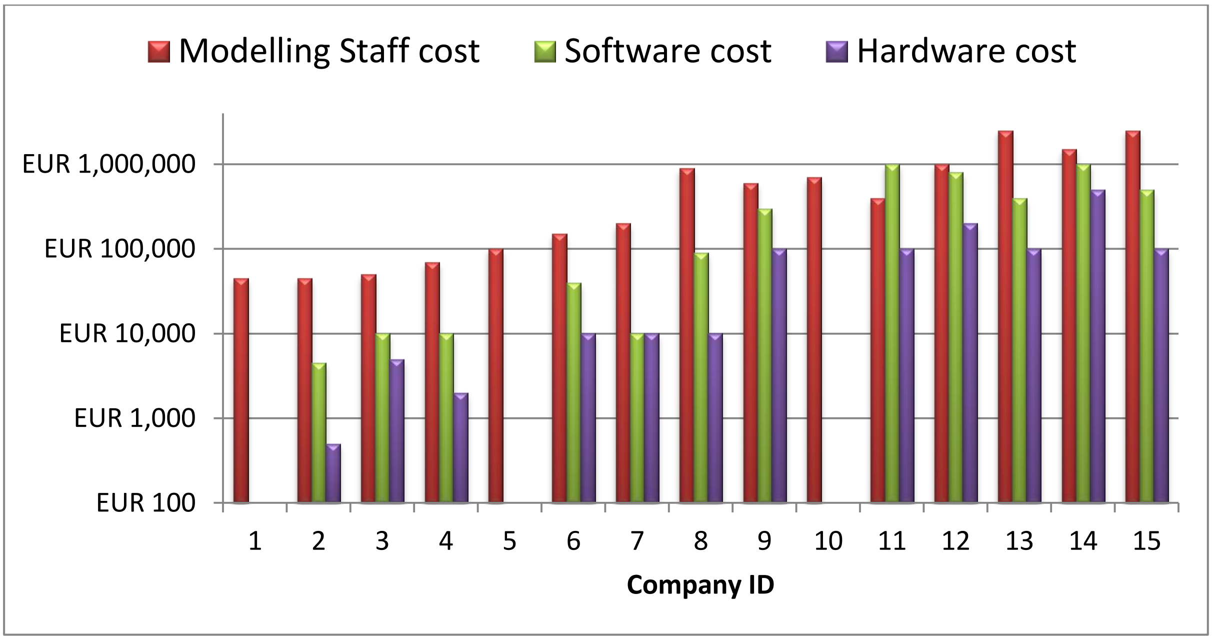
Figure 14 shows the cases where both the total and materials modelling investment were available. A wide variety of project sizes are represented, with total R&D investment ranging from €45K to €100M, with an average of €10M and a median of €1M. While the order of magnitude of investment is similar as shown on the log plot, there are basically two groups: (a) projects with a dominant modelling component (modelling takes 50% or more of the investment) and (b) projects where the cost of modelling part is 10% or less of the total R&D project investment. The former is most likely a result of the type of survey whereas the latter seems more typical for an industrial R&D setting. For example, one respondent commented that modelling costs are ca. 10% of the total project costs.



Note: The ID given to a particular company varies across Figures.

Figure 14: Investment Ranges for different companies.

The investment in staff, shown separately in Figure 15 is typically the largest cost followed by software and hardware. Considering the cases that provide all three figures, the ratio of staff to median of software and hardware, respectively is 100/20/6.

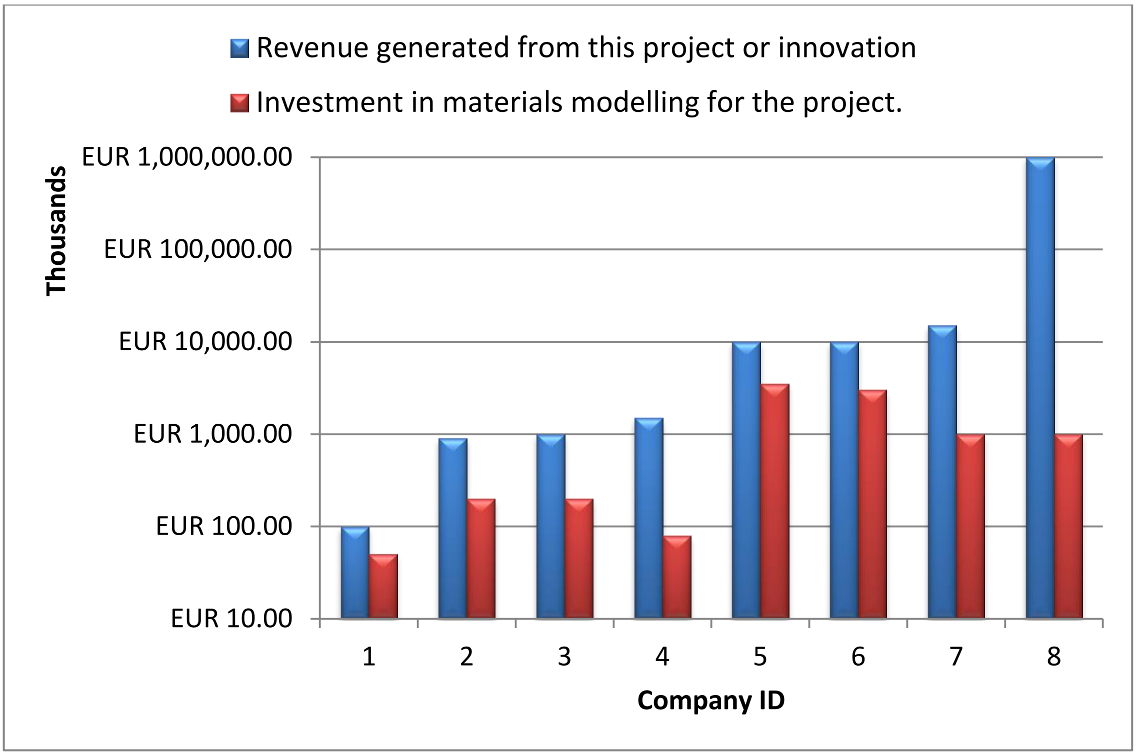


Note: The ID given to a particular company varies across Figures.

Figure 15: Investment by Type.

Actual or expected revenue generated from the project

Twelve responses were received from manufacturing companies. Four said that there was no revenue generation from the project, while for the other eight the revenue was between €100K and €1B (see Figure 16) with an average of €13M and a median of €5.75M.



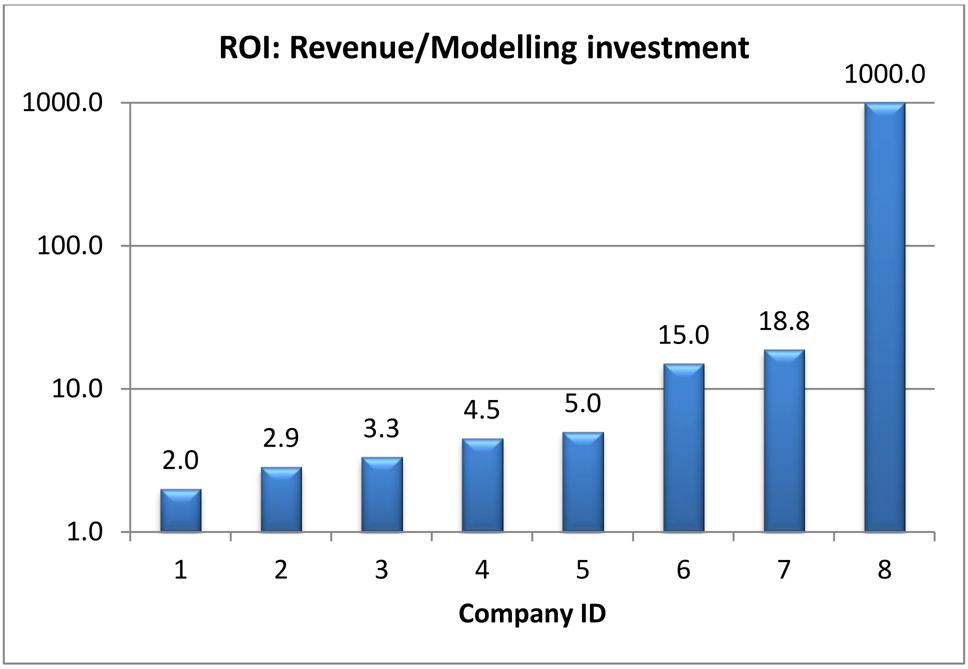
Note: The ID given to a particular company varies across Figures.

Figure 16: Revenue generated from the project and investment in materials modelling.

Return on investment

It is very difficult to determine the return on investment from a single activity in a complex innovation process. Here a very simple metrics is used, i.e. the ratio of the revenue generated from a product that was developed with the support of modelling and the cost of the modelling project. A similar ROI metric was used by IDC in a pilot study on the ROI of investing in High Performance Computing [24].

Eight companies provided both the investment in modelling and the total investment and revenue generated from the project. From these figures an ROI factor (ratio of revenue generated and investment in modelling) was determined. It ranged from 2 to 1000 (see Figure 17) with an average of 130 and a median of 5. Removing the largest and the smallest ROI yields an average of 8.



Note: The ID given to a particular company varies across Figures.

Figure 17: Return on investment (the ratio between revenue generated from products resulting from the project in which materials modelling was used and the investment in materials modelling).

There is also a trend for ROI to grow more than linearly with investments in modelling, as shown in Figure 18.

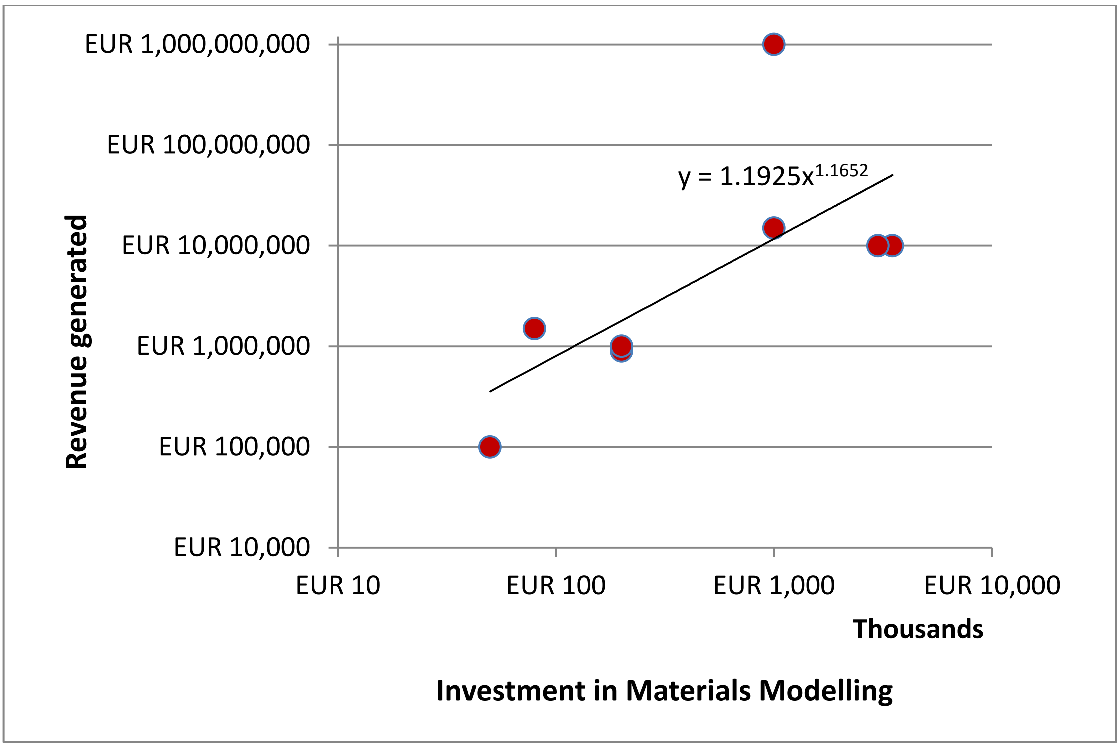


Figure 18: The chart depicts the increase in revenue with investment in materials modelling. The power law trend-line shows a slightly above linear increase.

The findings are consistent with those of the IDC pilot study on HPC [24]. The IDC report provides an ROI figure based on the revenue per investment into HPC (i.e. not including software and staff costs carrying out the project). For comparison we have to consider relevant industry segments such as manufacturing industry, for which the reported ROI is 28.1, averaged over 13 cases (see Table 4 of the study). A more detailed comparison can be made by considering the case data provided by IDC in connection with the study. We found 11 engineering applications in manufacturing as well as oil and gas segments. The projects included the following applications of HPC:

- Seismic data processing and analysis
- Innovative Engineering in Race Car Design
- Optical encoder design
- Manufacturing simulations
- Optimized and innovative data analytics
- Maximizing oil reservoir production
- Depth imaging in exploration

The ROI (revenue/HPC investment) for these 11 HPC cases in engineering ranges from 4 to 1350 with an average of 188 and a median of 43.

For comparison, the ROI (revenue/hardware cost) for the eight materials modelling cases is significantly larger, ranging from 20 to 10,000 with an average of 1400 and a median of 95.

Conclusions and outlook

Materials modelling and the resulting advances in materials and products manufactured from these materials have the potential to impact the economy and society in a variety of ways. This study briefly delineated the types of metrics and methodologies that can be used to quantify the economic impacts of materials modelling from a variety of perspectives including R&D stakeholders, industry stakeholders, and society. The study also investigated how materials modelling impacts the industrial R&D process and outlined the value and potential of materials modelling for industrial research and innovation, competitiveness, and profitability using examples from both the pharmaceutical industry and the molecular modelling industry. Finally, results from a survey of manufacturing organisations were presented. Based on responses of more than 30 companies, a wide range of key performance indicators for R&D process improvements and business enhancements could be determined. It was also possible to carry out some quantitative economic analysis including investments made into staff, software, and hardware, job creation, and revenue generation. Evidence for substantial ROI was found, corroborating the findings of earlier studies.

At the same time, it is noted that some of the companies that responded had been involved in materials modelling projects but did not see the need or benefit of using materials modelling in-house. They represent a sector of industry that has adopted a wait and see approach. Hence, there is a need to address this gap and ensure that the benefits clearly demonstrated in this report can be realised by a much larger range of organisations, an issue elaborated in detail in the EMMC Roadmap for Materials Modelling [21].

Appendix: UK REF exercise

The following are excerpts from the Case Studies submitted to the 2014 UK REF exercise. See http://impact.ref.ac.uk/CaseStudies/Search1.aspx to search all case studies.

Design for manufacture and reliability of microsystems (University of Greenwich, Electrical and Electronic Engineering, Metallurgy and Materials) The Computational Mechanics and Reliability Group at the University of Greenwich has been developing design and materials modelling expertise and tools for electronic manufacturing and reliability since the late 1990s. This case study details economic and environmental impacts and impacts on practitioners. In particular it shows how our expertise has: substantially aided companies to assemble miniaturised electronic systems using environmentally friendly materials; aided companies to predict reliability of new electronic systems before physical prototyping providing significant cost savings; led to formation of spin out companies by our academic partners.

Advanced Materials Modelling for Earth and Space Application (University of Greenwich, Electrical and Electronic Engineering, Metallurgy and Materials) Research in materials modelling by the Computational Science and Engineering Group (CSEG) is helping aerospace, defence and transport companies design advanced materials and new manufacturing processes. From lightweight components like aeroengine turbine blades to the control of magnetic fields to stabilise the next generation of International Space Station levitation experiments, CSEG is supporting innovations which have economic impact due to increase in competitiveness, market share, energy cost reduction and better use of raw materials; environmental impact due to new lightweight recyclable materials and reduced energy processes; increased public awareness of the importance of advanced materials and influenced government policy. In the assessment period, CSEG collaborated closely with leading industries in steel-making (ArcelorMittal, Corus), primary aluminium (Dubal, Rusal, Norsk-Hydro, SAMI) and lightweight structural materials for transport and aerospace (European Space Agency, Rolls-Royce).

Fluid Modelling - Expertise and Software (Sheffield Hallam University, Electrical and Electronic Engineering, Metallurgy and Materials) Fluid modelling approaches devised by the Materials and Engineering Research Institute's (MERI's) materials and fluid flow modelling group have impacted on industrial partners, research professionals and outreach recipients. This case study focuses on economic impacts arising from improved understanding which this modelling work has given of commercial products and processes. These include: metal particulate decontamination methods developed by the UK small company Fluid Maintenance Solutions; liquid crystal devices (LCDs) manufactured by the UK SME ZBD Displays; and an ink-droplet dispenser module originally invented at the multinational Kodak. Additionally, the modelling group's computer simulation algorithms have been adopted by industrial research professionals and made available via STFC Daresbury's internationally distributed software

package DL_MESO. Finally, the group has developed, presented and disseminated simulation-based materials and visualisations at major public understanding of science (PUS) events.

Improved Creep-Fatigue-Oxidation Resistance in Gas Turbine Disc Materials (University of Portsmouth, Aeronautical, Mechanical, Chemical and Manufacturing Engineering)

Research at Portsmouth has significantly improved the understanding of damage tolerance under creep-fatigue oxidation conditions experienced in aero -engine components. The understanding has been developed through research on new-generation disc materials including U720Li and RR1000, which have since been used in Rolls -Royce engines including Trent 900 in Airbus A380, Trent 1000 in Boeing 787 and the latest Trent for Airbus A350 XWB. These new materials have enabled aircraft to operate more efficiently at higher temperature with a major impact on CO 2 emission and a significant impact on economy due to the new market opportunities and reduction of operating costs.

Structural science – equipment and software for industry (University of Durham, Chemistry Department)

Durham Chemistry has a long history of research in cutting edge crystallographic methods and innovative instrument design which has led to the commercialisation of scientific apparatus and software with significant sales value. Durham-developed apparatus and crystallographic software are used globally by both industry and academia. Autochem2, for example, is sold exclusively to Agilent via the spin-out company OlexSys, and hundreds of researchers rely on Durham's contributions to the Topas software package. Crystallographic research for pharmaceutical and other companies, research-based consultancy, commercial analytical services and provision of international PhD+ level training schools have led to further significant impact.

Commercialisation of materials modelling software (CASTEP) (University of Durham, Physics Department)

Durham researcher, Prof Stewart Clark, is one of the six original co-developers of the Castep software package which calculates the electronic, physical and chemical properties of materials from first principles. CASTEP was written to solve a variety of research problems from semiconductor devices and liquid crystal displays, to the behaviour of Earth minerals under very high pressure, molecular dynamics and biological systems. The software package was commercialised for use in industry under license by Accelrys Inc., where it is bought and used by ~1000 high-tech companies for development of new materials in chemical, pharmaceutical, auto and jet engine manufacturing industries. Total sales revenue for Accelrys from the CASTEP code is in excess of $30M.

Robust design of micro-scale piezoelectric actuators (Brunel University, Aeronautical, Mechanical, Chemical and Manufacturing Engineering)

The research produced accurate simulation models of piezoelectric actuators for investigating sensitivities to parameter variations that led to maximum power for minimum electric field. This was the basis of design rules for determining new products at the industrial partner NXT, now named Hi-Wave Technology, headquartered in Cambourne, UK. Old design rules had led to two failed products whereas these new design rules have guided successful products with a major Japanese television manufacturer, a Japanese printer company and a Russian mobile phone company. Without this research Hi-Wave would have stopped activities in this technology. To date, licences for more than 24 million units per annum have been sold and more than 280,000 units manufactured.

Realising innovative and adaptive product design and optimisation through an integrated materials and modelling system (Liverpool John Moores University, Aeronautical, Mechanical, Chemical and Manufacturing Engineering)

The investigators of this impact case study have utilised their expertise in materials engineering, theoretical/numerical modelling and product development to achieve significant economic, social and environmental impacts in a range of fields through developing a systematic methodology for innovative product design and optimisation. Through several industrial projects and collaborations, significant impacts have been witnessed including new products creating several million pounds in revenue annually for businesses in different sectors and green manufacturing technologies in repair and reclamation of components. All the described impacts were results of investigation in the Mechanical Engineering and Materials Research Centre (MEMARC) over the assessment period.

The research work in MEMARC has been conducted by effectively integrating materials engineering, theoretical/ numerical modelling and product development through intensive collaboration with industrial partners from different sectors. The main research activities included the development of a novel material characterisation methodology and the modelling of materials at different scales such as atomic level, crystal nucleation and microstructure

CASTEP (University of Cambridge, Physics Department)

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.

High Performance Magnesium Alloys (University of Manchester, Metallurgy and Materials)

Research at Manchester has led to the development of a new class of high performance magnesium alloys based on the addition of rare-earth alloying elements. The new alloys combine low density and the highest strength of any magnesium alloy. Used to substitute for aluminium in aerospace and automotive they produce weight savings of 35% improving performance and reducing fuel consumption. Commercialisation of these alloys by Magnesium Elektron (ME), the international leader in magnesium alloy development, contributes over $20m per annum to company revenue. This includes development of the first commercial product available for bioresorbable magnesium implants, SynermagTM, launched in 2012.

Enabling Zyvex Labs to develop atomically precise manufacturing processes (University College London (UCL) Physics)

The underpinning research involved modelling the diffusion of hydrogen on silicon surfaces, and the electronic structure of dopant atoms on silicon surfaces. This data was used to inform, guide and develop the atomically precise manufacturing processes of Zyvex Labs. These processes remove hydrogen atoms from a silicon surface to create patterns with atomic precision for later overgrowth. As a result of the UCL research, Zyvex Labs has already obtained funding of $14 million, several jobs have been created, and at least two products are being brought to market.

Enabling SEMATECH and industrial member companies to improve their transistor technology (University College London (UCL) Physics)

Researchers within the Department of Physics and Astronomy at UCL have investigated the properties of defects in bulk HfO2 and at Si/SiOx/HfO2 interfaces. Results have been used by an industrial partner, SEMATECH (SMT), to improve the quality and reliability of high-performance microelectronic devices based on transistors. This has helped SMT to meet project objectives on behalf of member companies such as Intel and IBM, and UCL research results have been consistently highly evaluated by these companies. Recommendations made by SMT have been implemented by industrial partners in their currently manufactured devices, such as the 22nm process technology released by Intel in 2011.

MOLPRO – A Quantum Chemistry Package (University of Birmingham, Chemistry Department)

Work at Birmingham by Peter Knowles and Fred Manby on improving the efficiency of calculating integrals for so-called ab initio calculations, widely used in computational chemistry, has led to a novel, fast algorithm for the accurate calculation of molecular energies and structures. It contains a level of theory, known as MP2, widely used in modelling by industry (pharmaceutical and chemical) as well as in academia. The new local approximation of the method, DF-LMP2, was developed at Birmingham and implemented in the MOLPRO package that has been sold worldwide, generating economic impact. A major attraction of the package is that MOLPRO can do a range of calculations efficiently, MP2 being one of them.

The impact from MOLPRO in the REF window has been primarily economic and can be quantified through sales of MOLPRO to academia and industry throughout the REF window, as follows (data provided by Cardiff University): £1,783,714 (January 2008 – July 2013). The main contributors to the economic impact are academic users but just over 10% have been commercial users and companies, contributing £203,480, as of 31 July 2013. These include organisations such as Cilag AG (a Swiss pharmaceutical firm), BASF, Hitachi, Nissan Chemical Industries, DE Shaw Research (a computational biochemistry research company) and Schrodinger (a software company).

Evidence for the impact of MOLPRO on facilitating research by commercial users includes that from BASF. BASF conducts research into fields such as theoretical chemical modelling as part of its ongoing product development process, which requires a high-performance computing (HPC) platform. A Group Leader in Quantum Chemistry at BASF and current user of MOLPRO states:

"MOLPRO and in particular its capability for very accurate computations on large molecules, has become a valuable tool for estimating thermochemical and kinetic data for substances and reactions involved in our development of new materials and processes."

Materials modelling using ab-initio electronic structure calculations (University of York, Physics Department)

A computer program, CASTEP, has been developed to use quantum mechanics to calculate the structure and properties of materials. The code is distributed commercially via Accelrys Inc. with sales, for example, in the automotive, electronics and pharmaceutical industries in excess of £1m per year since 1998, accelerating to over £2.5m per year recently and total sales (late 2012) exceeding $30m. Commercial applications include designing new battery materials and electrodes to improve the performance of electric cars (Toyota), integrating organic electronic materials for light-weight flexible displays (Sony), and developing new catalysts for hydrogen-powered fuel cells (Johnson-Matthey).

Examples of CASTEP-based patent applications show two automotive uses of CASTEP: for developing new catalysts for vehicle exhausts, and new solid battery electrolytes:

[i] Patent EP1243329A1 "Ceramic body and ceramic catalyst body" (issued 2008);

[ii] Patent EP2555307 "Sulfide solid electrolyte material, battery and method for producing sulphide solid electrolyte material" (filed 2010)

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