The Economic Impact of Materials Modelling

Indicators, Metrics, and Industry Survey

Gerhard Goldbeck, Goldbeck Consulting Ltd
Christa Court, MRIGlobal

Background

- EMMC and International Materials Modelling Board (IM2B)
- Co-authored by Christa Court (Economist) MRIGlobal
  - Context: MRIGlobal provides cost-benefit analysis for energy planning and research infrastructure support at the National Energy Technology Laboratory (NETL)
- Report available at https://zenodo.org/record/44780
- *Financial support by European Commission and University of Cambridge is gratefully acknowledged.*

NETL Computational Modelling Research

- Funded by U.S. Department of Energy, National Energy Technology Laboratory, Crosscutting Research Program
- Assess the economic impacts of NETL computational modelling efforts
- Performed qualitative and quantitative assessments of two open source models related to multi-phase flow modelling and computational chemistry.
- Lessons Learned:
  - Data needed to assess economic impacts directly are rarely collected or estimated during model development and/or distribution
  - Case studies on individual models are possible but generalizations to economic impacts of other types of modelling are limited
  - Full economic impact analysis is not possible under the time and budget scope set aside for this type of work.

Impacts of new technologies

- Benefits as well as costs (winners and losers)
- What types of impacts to measure?
  - Impact of R&D spending, deployment or availability of new software/materials?
- What is the scope of the impact measurement? Impacts on …
  - software or material developer industry,
  - manufacturing industry, whole economy
  - Local, national, regional, international?
  - Societal impacts?

Challenges of macro-economic impact assessment

- Materials Modelling is a disruptive technology: changes the ‘supply side’
  - Economic accounting-based methods used for most standardized impacts assessments are not ideal
- Dynamic simulation models are more appropriate but do not exist in a standardized form.
- Appropriate econometric modelling will be scenario specific and necessitate someone with a high level of domain knowledge in both fields.

Micro-economic impacts

– Currently used simple Return-on-investment models

– cost-benefit analysis requires much more detail

Assessing the impact of materials modelling research

- Publications and patents
- Growth of populations of beneficiaries of modelling such as users of models and end-users of modelling results
- Acceptance levels of materials modelling by peers in industry
- Simple macro-economic impact models
- Case Studies: https://materialsmodelling.com/2016/04/26/industry-case-studies-combining-discrete-and-continuum-modelling-to-address-industrial-rd-challenges/

Reports

The economic impact of molecular modelling

http://gerhardgoldbeck.wordpress.com/2012/07/10/the-economic-impact-of-molecular-modelling-of-chemicals-and-materials/

Industry interactions of the electronic structure research community in Europe

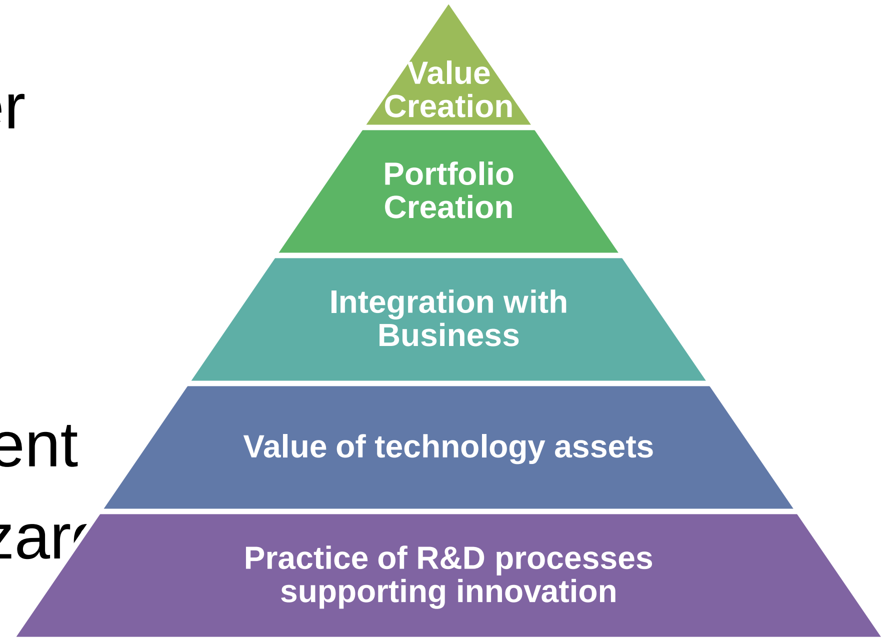
http://gerhardgoldbeck.wordpress.com/2014/01/20/industry-interactions-of-the-electronic-structure-research-community-in-europe/

R&D process improvement

Mechanisms:

- More efficient experimentation
- Broader Exploration and Deeper Understanding
- Saving a Product Development Project
- Accelerated Product Development
- Improved safety testing and hazard avoidance
- ROI of 3:1 or more

M. Swenson, M. Languell, and J. Golden, “Modeling and Simulation: The Return on Investment in Materials Science,” IDC, Jun. 2004.



T. D. Parish, “The Technology Value Pyramid,” Ch.5 in: Assessing the Value of Research in the Chemical Sciences, Washington: Academies Press, 1998.

Efficient Experimentation	Low	High	Updated
Cost per experiment	13000	13000	13000
Experiments per project	10	10	10
Number of projects impacted	4	18	10
Reduction on experimentation	15%	35%	50%
Benefit	78,000	819,000	650,000
ROI	1.56	2.34	**2.81**
Innovation due to broader exploration	Low	High	Updated
Total market size for product category	100,000,000	100,000,000	100,000,000
Market share increase resulting from project	1%	1%	1%
Percentage of Projects Generating a Product Improvement	7%	20%	20%
Number of projects impacted	4	18	10
Contribution from modelling	15%	15%	15%
Benefit	42,000	540,000	300,000
ROI	0.84	1.54	1.30
Saving stalled projects	Low	High	Updated
Percentage of projects saved	0.20%	1.25%	1%
Value of save, Development cost per project	6,500,000	6,500,000	6,500,000
Number of projects impacted	4	18	10
Benefit	52,000	1,462,500	812,500
ROI	1.04	4.18	**3.52**
Risk Management Through Safety Testing	Low	High	Updated
Percentage of Projects with a Hazard or Safety Element	1%	3%	3%
Value of Hazard or Liability Avoidance	2,000,000	2,000,000	2,000,000
Number of projects impacted	4	18	10
Benefit	80,000	1,080,000	600,000

ROI of materials modelling

DIRECT BENEFITS	Low	High	Updated
More efficient experimentation	78,000	819,000	650,000
Broader exploration	42,000	540,000	300,000
Saving stalled projects	52,000	1,462,500	812,500
Risk management	80,000	1,080,000	600,000
Potential TOTAL DIRECT BENEFITS	252,000	3,901,500	2,362,500
DIRECT COSTS	Low	High	Updated
Software licenses	35,000	90,000	40000
Hardware	6,000	100,000	30000
Training	7,000	2,000	3000
IT support	2,000	8,000	8000
Labour	0	150,000	150000
TOTAL DIRECT COSTS	50,000	350,000	231,000
ROI estimate	**3**	**9**	**7**

Performance metrics for a modelling function in R&D: Define and Monitor Impact Levels

Level 1a: Data

Chemistry/physics/materials data

↓

Level 1b: Analysis

Application of materials modelling (incl scientists, software, hardware)

↓

Level 2: Scientific Decision Support

Guidance on next steps, screening lists, experiment selection

↓

Level 3: Programme Impacts

Improved materials/processes/components

Bristol-Myers Squibb 2011

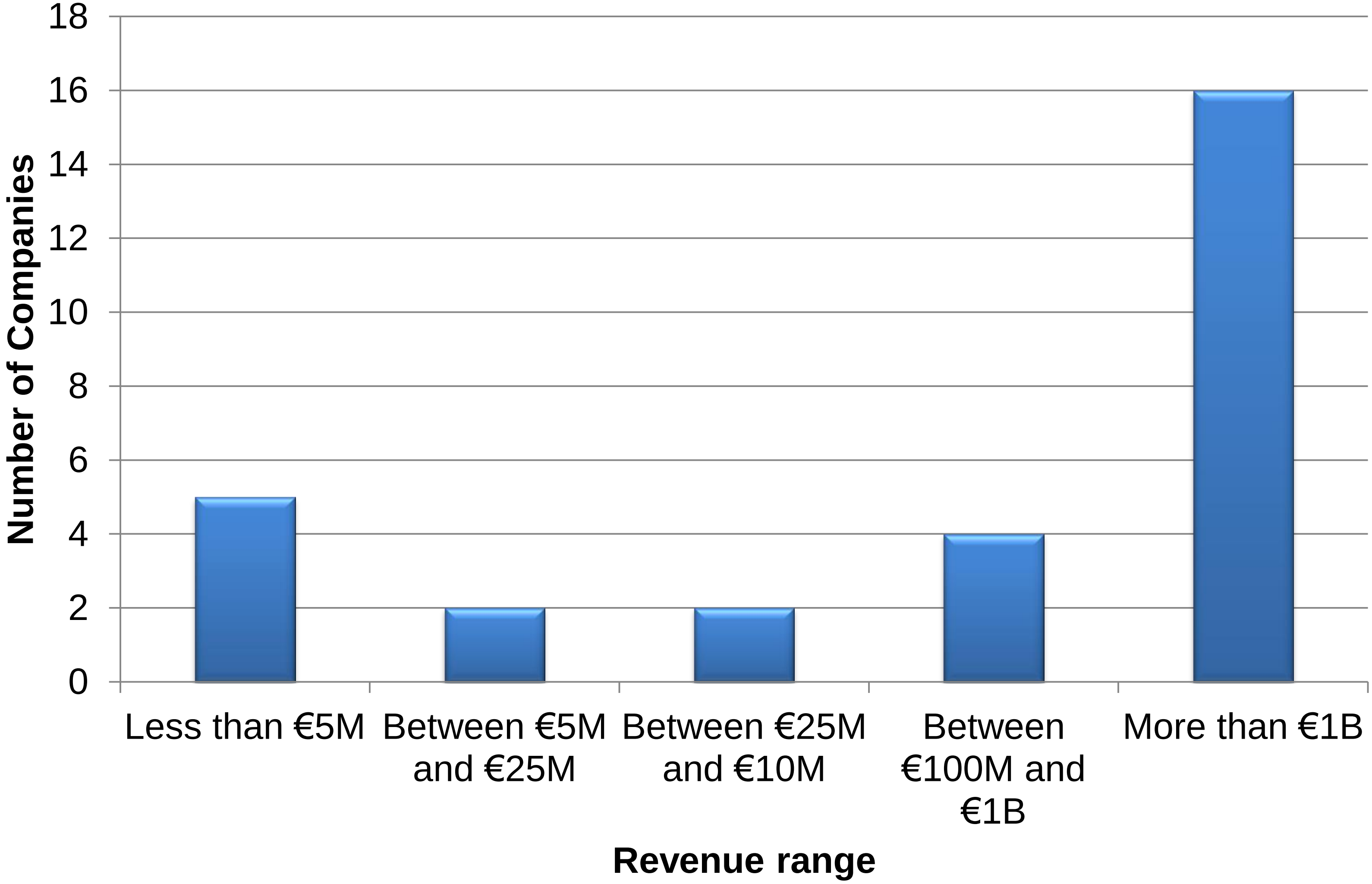
Outcomes: maximise value

- 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.
- Deeply involved, focused, support is more impactful than in-and-out work.
- Focus innovation projects on improving observed issues

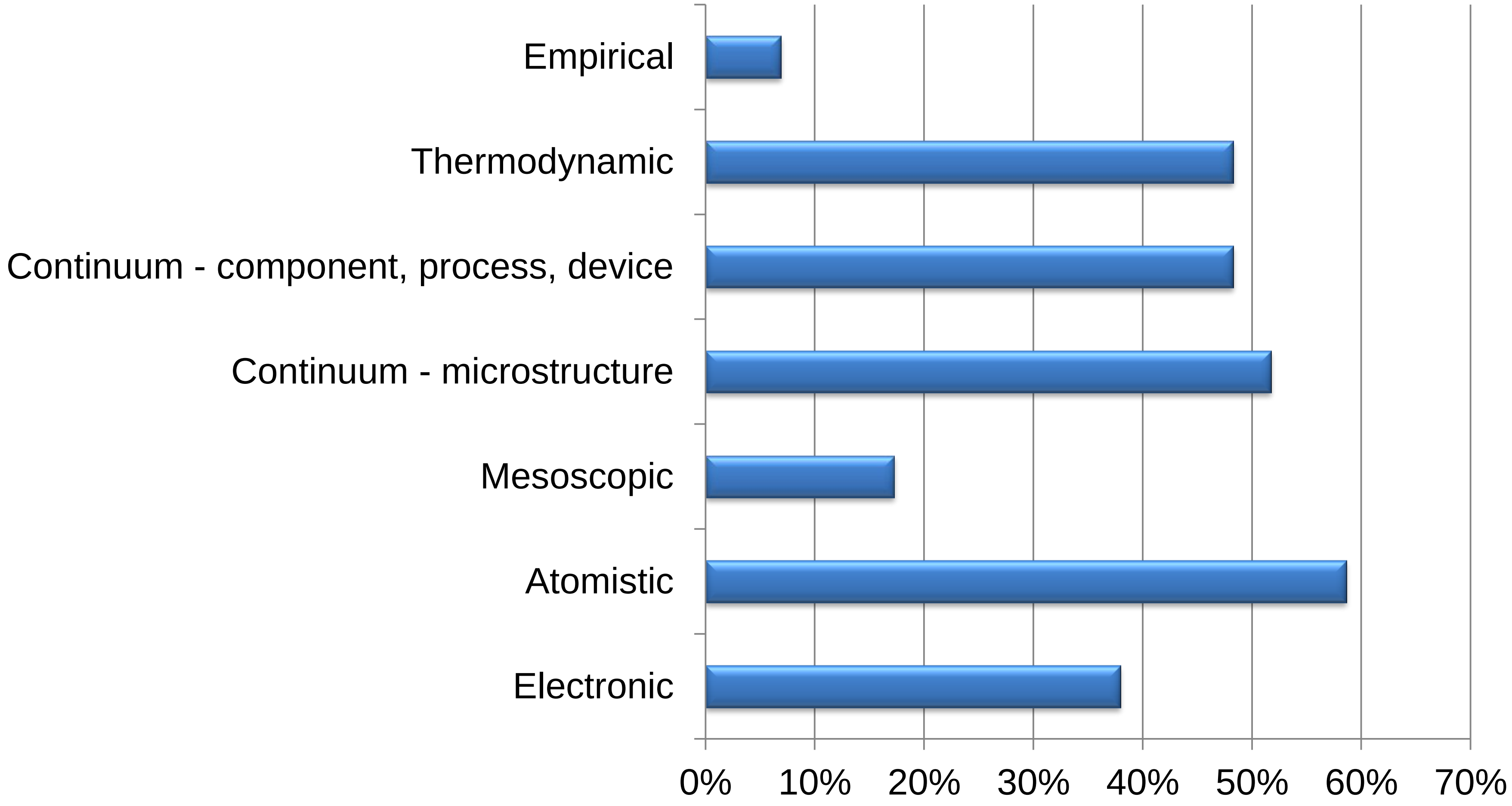
Economic Impact Survey

- 150 manufacturing organisations invited.
- 34 responses from manufacturing organisations were obtained representing a response rate of about 23%.
- 5 responses were from manufacturing companies that have been involved in materials modelling projects but do not carry out materials modelling within the organisations.
- 29 responses used for further analysis.

Respondents profile



Types of materials modelling used



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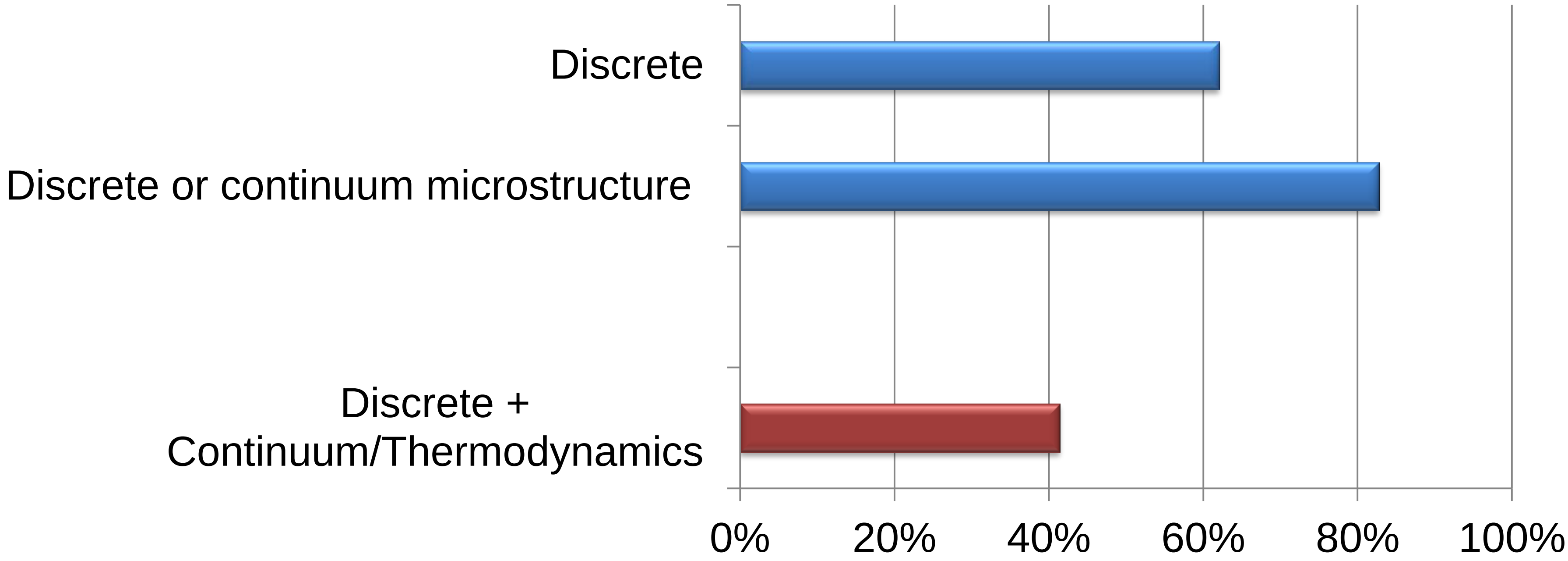
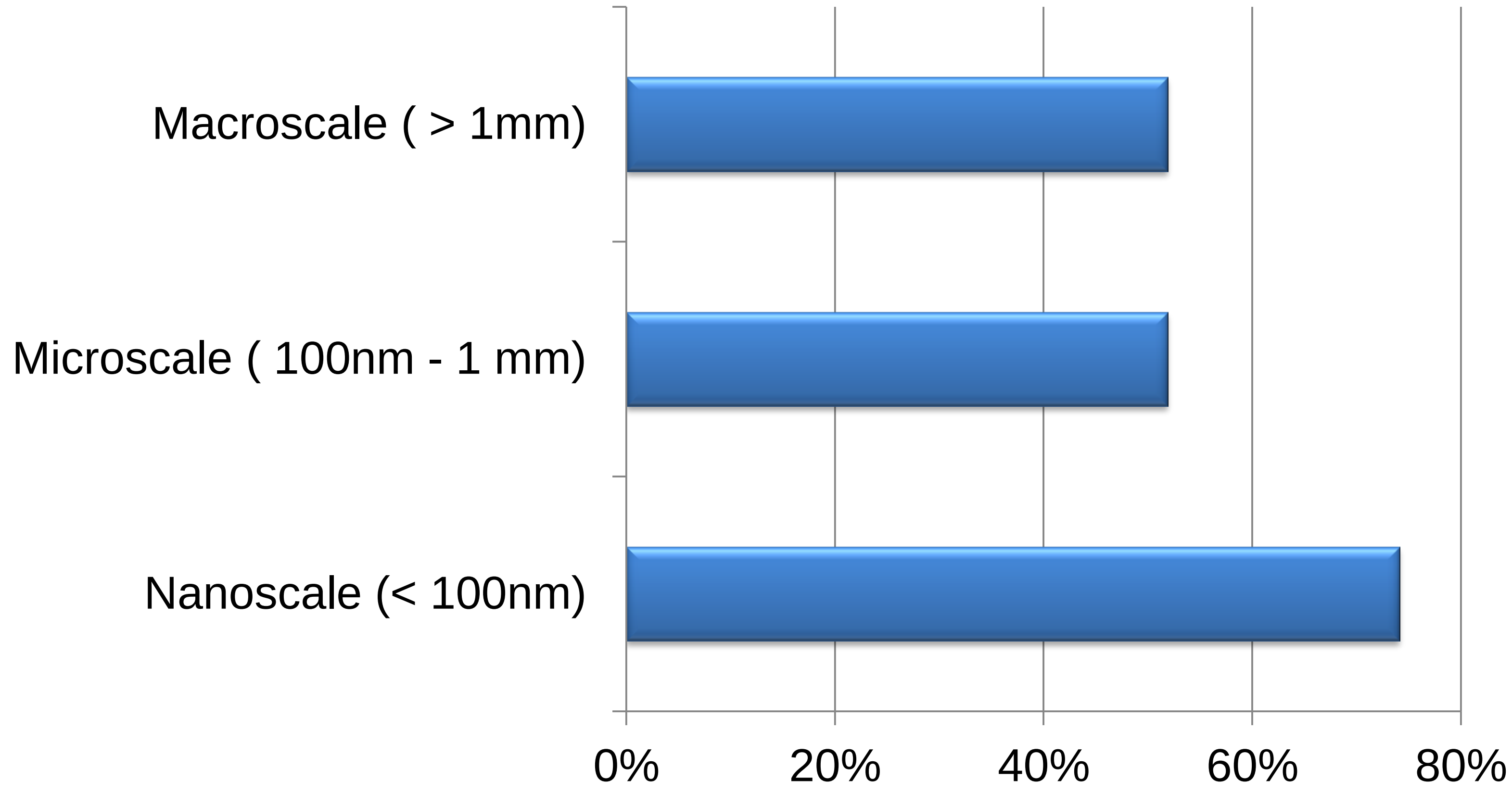
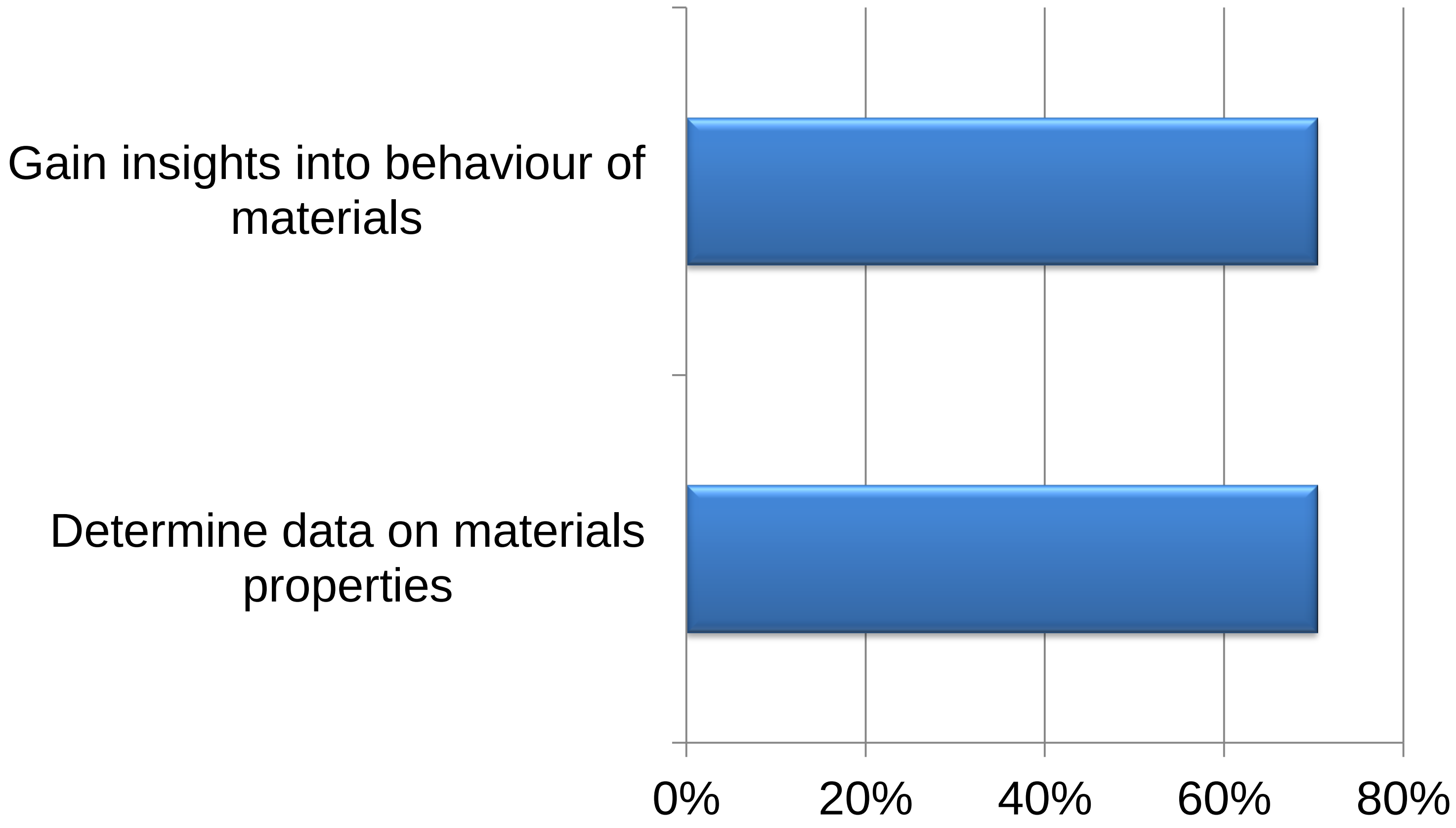


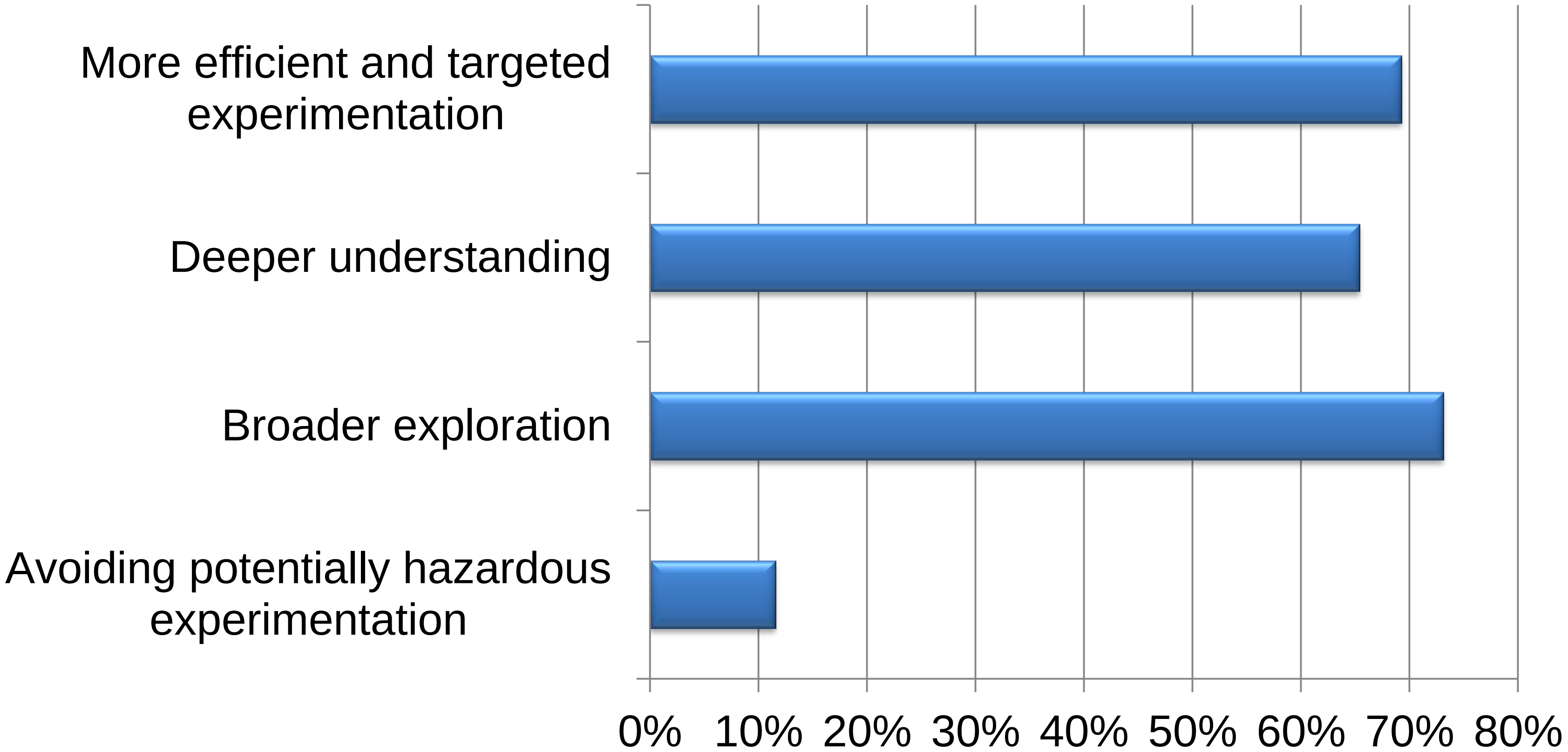
Scales investigated



Discovery modes



R&D process improvements



Technical and business performance indicators

- R&D process improvements
- Performance improvement/optimisation of formulation, product and process
- Explain differences in material performance that standard test method could not distinguish.
- R&D Strategy
  - Modelling helps to determine whether a target performance is easy to reach, just doable, or impossible.
- Underpinning intellectual property (IP), supporting patents and staking a wider claim.

Technical and business performance indicators

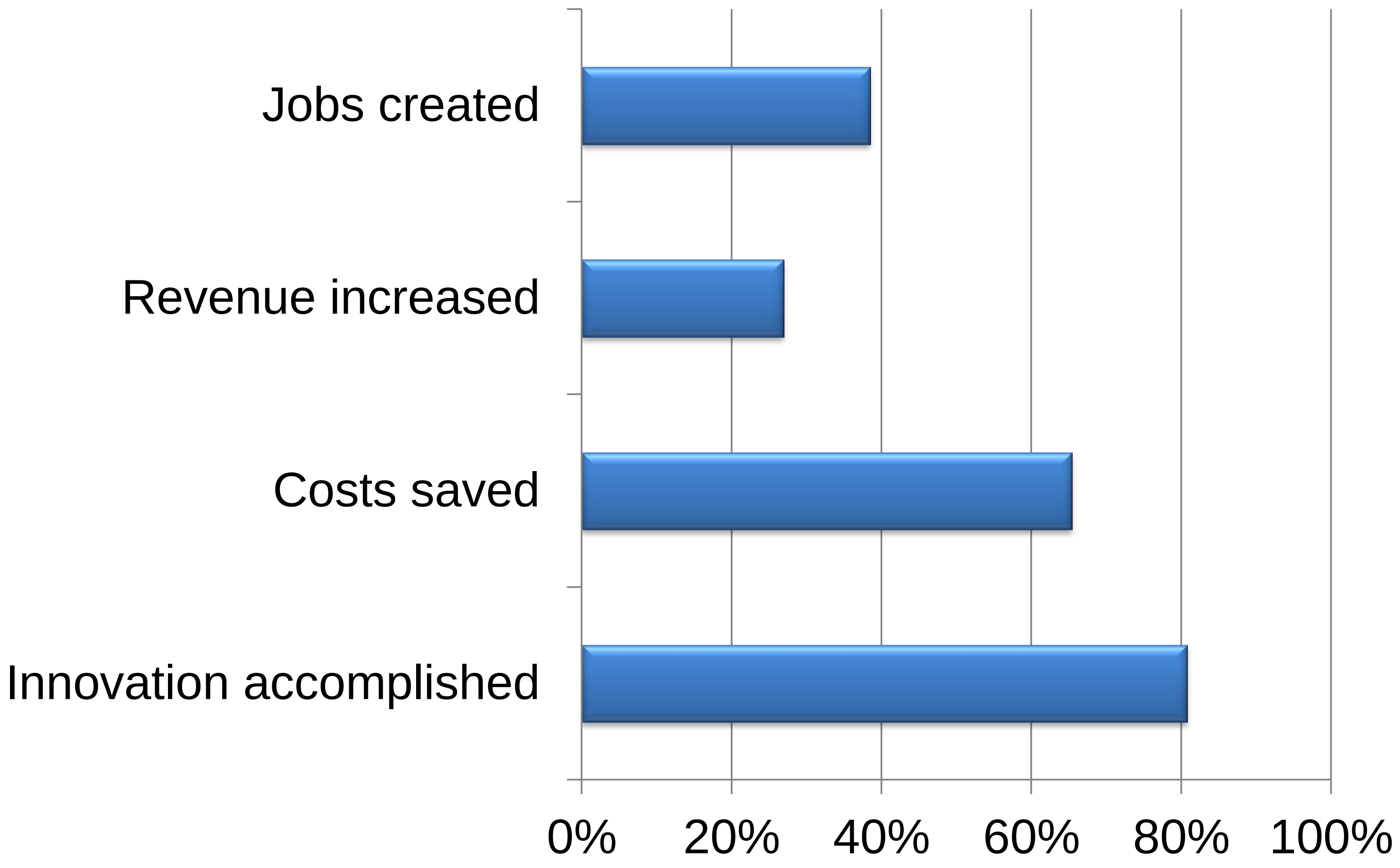
- **Engineering & Upscaling benefits**
  - Modelling as a bridge between process engineers at the production site and researchers in the R&D centre
  - Providing the level of detail in know-how about the product that lowers the technical risks of upscaling and market introduction
  - Providing the missing link between small scale material testing and large scale application results
  - Modelling allows testing and verifying new manufacturing strategies that were not physically available at the time.
  - Detailed process understanding resulting from modelling supports a faster and more assured market introduction.

Technical and business performance indicators

- ***Supplier-Manufacturer value chain***
  - 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

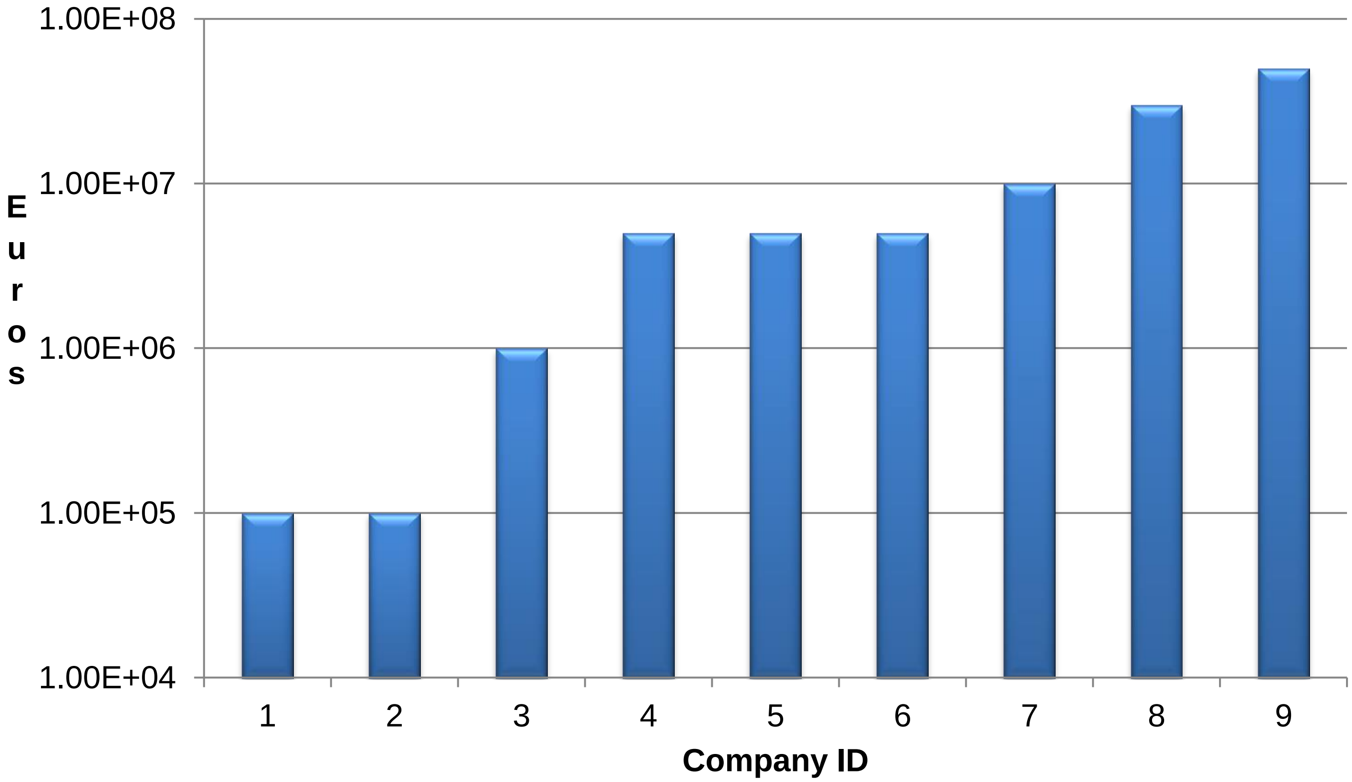
- ***Marketing and competitive benefits***
  - As a result of materials modelling the benefits of our materials compared to competitive materials could be demonstrated to customers.
  - A pedagogic and marketing tool to explain the technology through visualisation

Quantitative impact factors

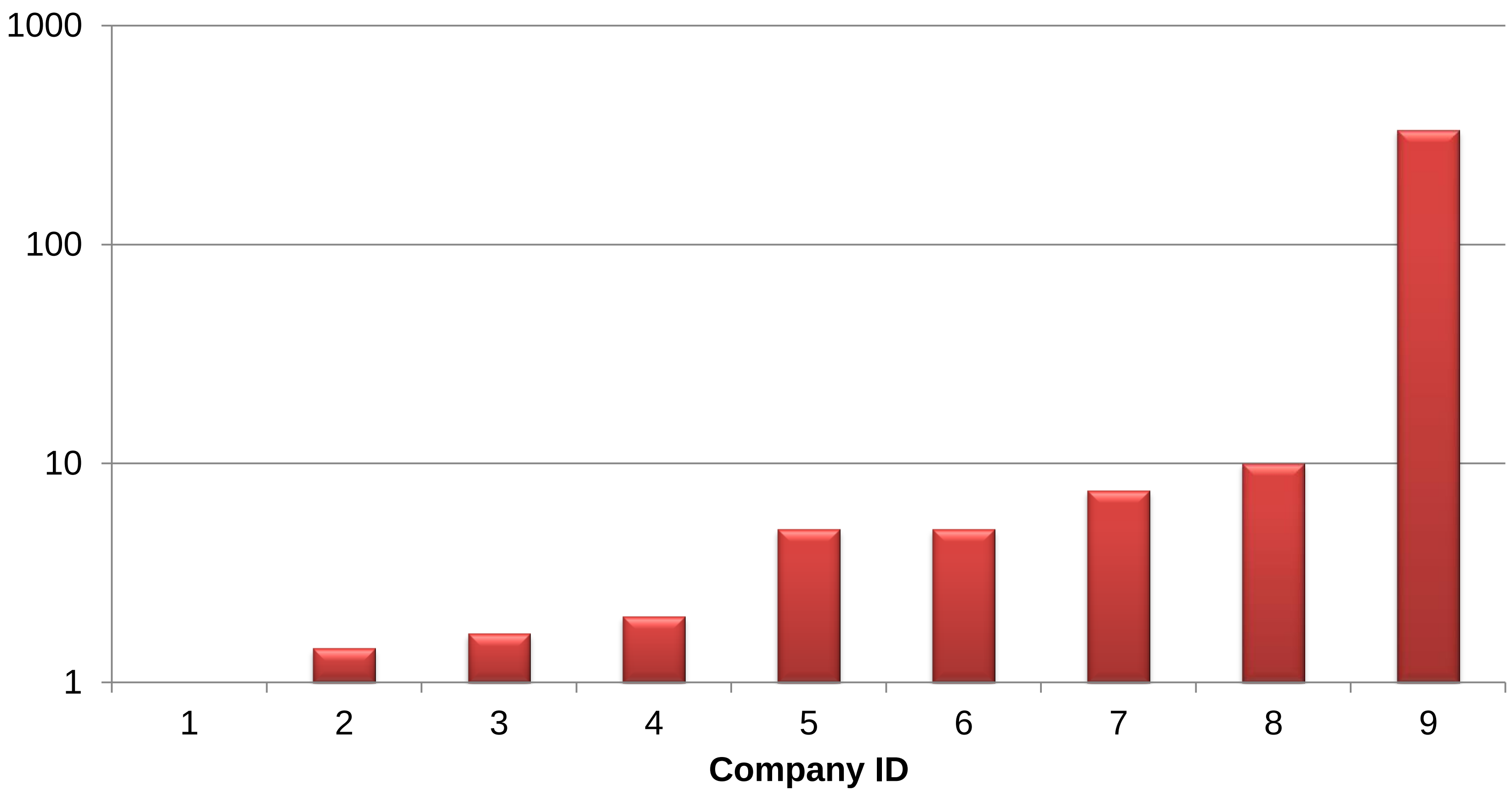


Cost saving

- 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.

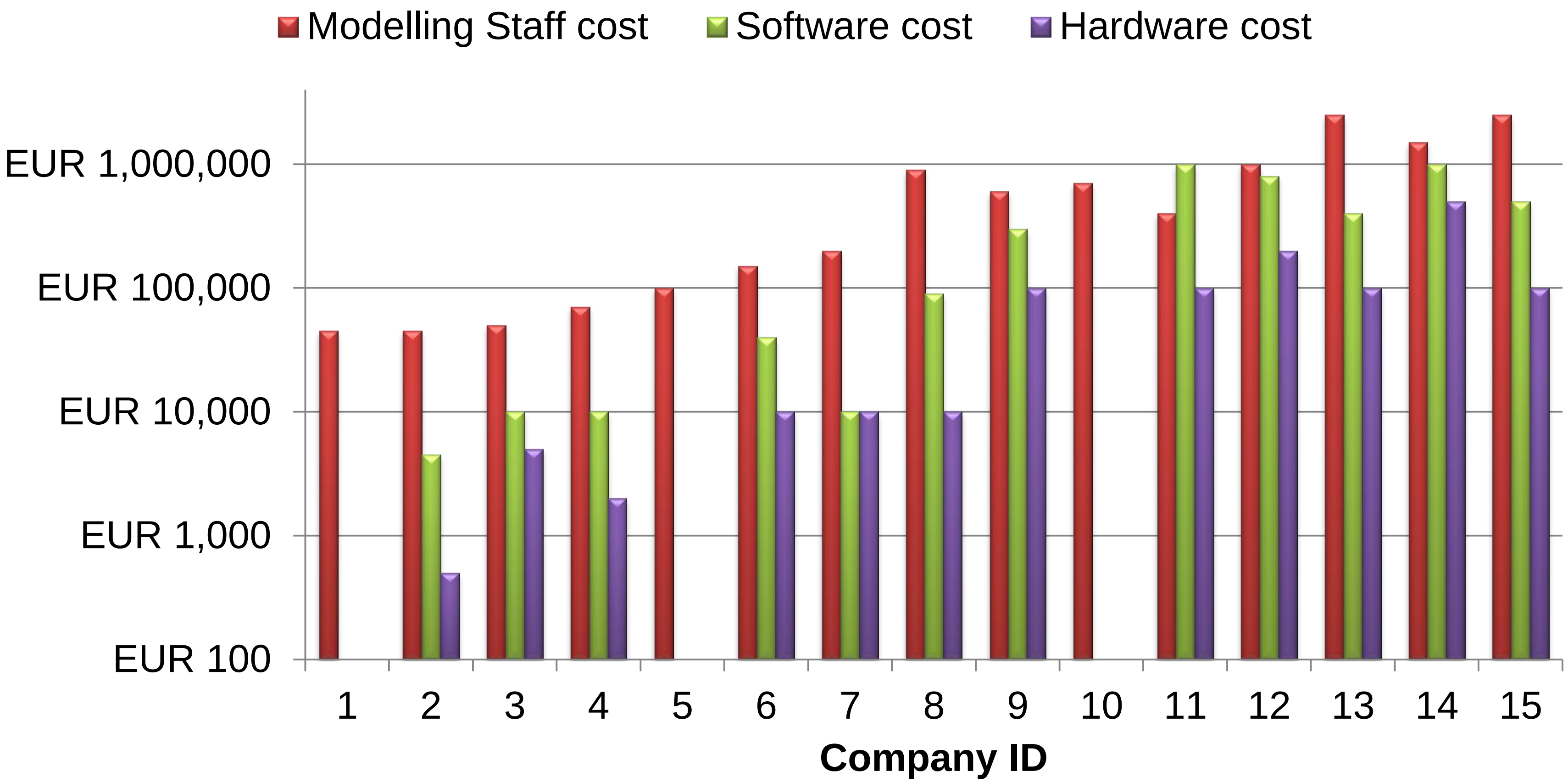


Cost saved/modelling investment

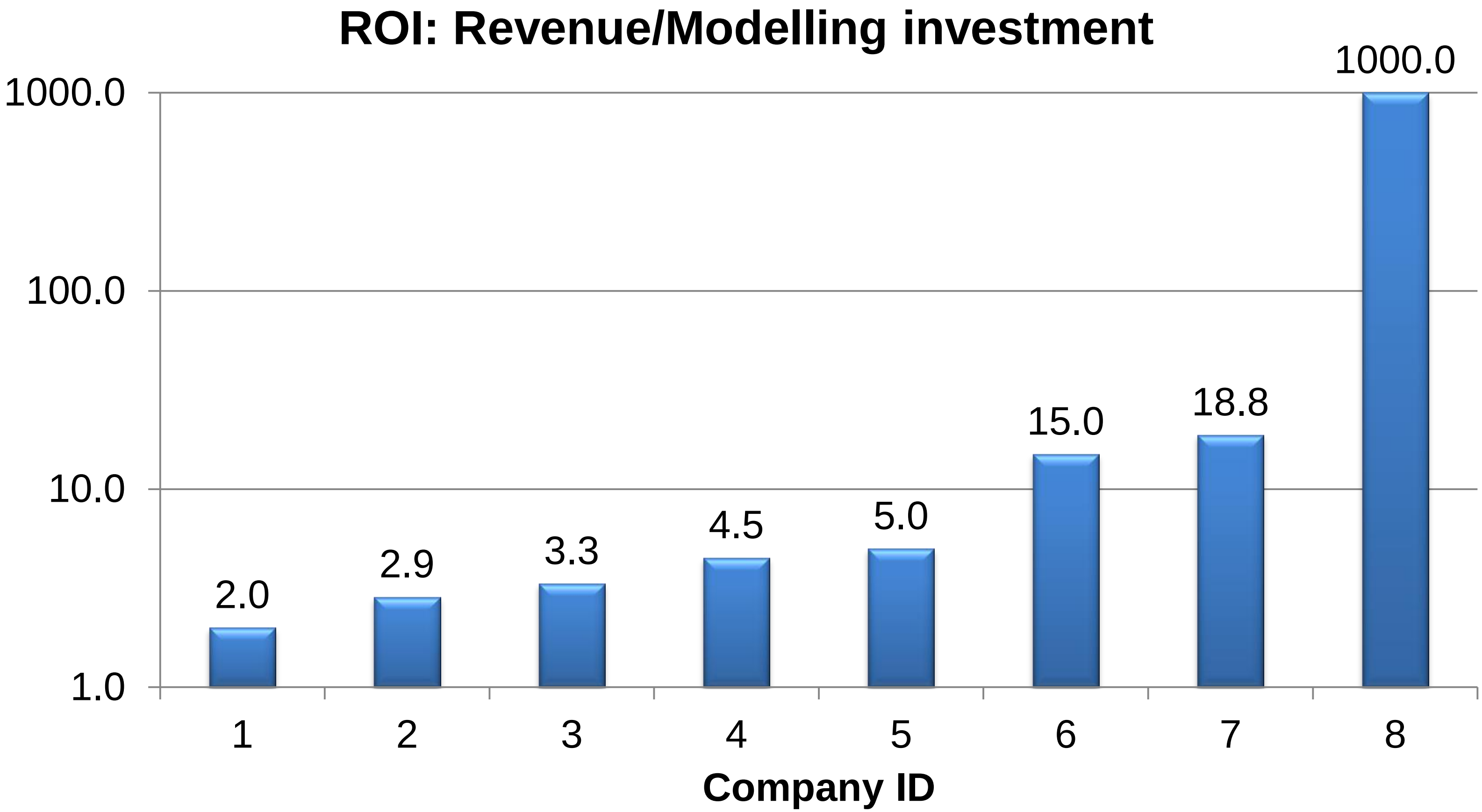


Investment

- Ratio of staff to median of software and hardware, respectively is 50/10/3



Return on investment



Widening Impact

- 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.
- 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.
- How can we get there?

Improving the attractiveness with SMEs

- In order for SMEs to adopt materials modelling (and realise many of the above impacts), developments are needed to
  - Identify key tasks and properties (in particular industry sectors)
  - Develop robust, easy to use tools.
  - Make the business case.

Making the business case

- Cost-benefit analysis needed.
- Gather data which would allow the reliable comparison between human, financial and time resources which have been spent for the product development with and without materials modelling.