Status of collected needs/key topics needing action in Europe

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European Materials Modelling Council (EMMC)

Outline

- Overall analysis of the survey
- Materials Model Development, enhance the use of discrete models, enhance coupling and linking, extracting materials properties from models, extracting the accuracy of different models, (Q1+2+3+4)
- Integration of materials models with manufacturing and processing (Industry 2020) (Q5)
- Integration of Materials Modelling in Business processes, (Q6)
- Materials Modelling Market Place and Dataspaces, (Q7)
- Integrated Workflows and Interoperability including experimental data (Q8)
- Coordinating network: Enhancing the uptake of material modelling by Manufacturers. (Q9)

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Overall analysis of the survey: Figures

EMMC Survey of materials modelling development needs

In this open survey you are invited to provide your views on what materials modelling developments are required in order to respond to the application needs of the European industry. The inputs collected via this survey will lay the groundwork for elaboration of the EMMC RoadMap 2018-2020, a process which will start during a meeting in Brussels on 20th May 2016, with participation (by invitation) of many active survey contributors.

The Open survey can be accessed under this link:
https://ec.europa.eu/eusurvey/runner/EMMC-materials-modelling-development

- More than 1500 stakeholders were invited to fill in this survey and we elaborated by feedback of more than **250 participants (20% are manufacturing industries and 40% software owners)**.

Survey analysis published on the https://emmc.info

EMMC Survey of materials modelling development needs: discussion notes towards the Road Map 2018-2020

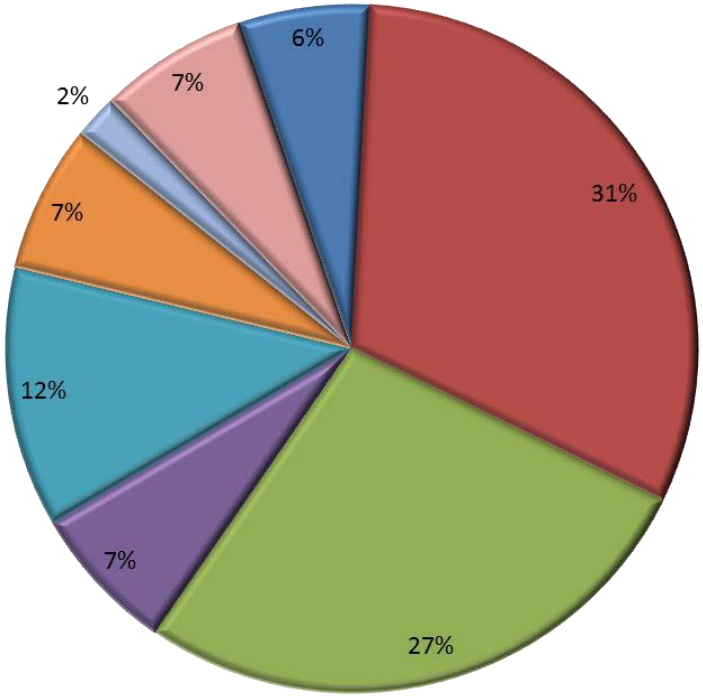
Authors (alphabetic order): Nadja Adamovic, Pietro Asinari, Gerhard Goldbeck, Adham Hashibon, Kersti Hermansson, Erich Wimmer

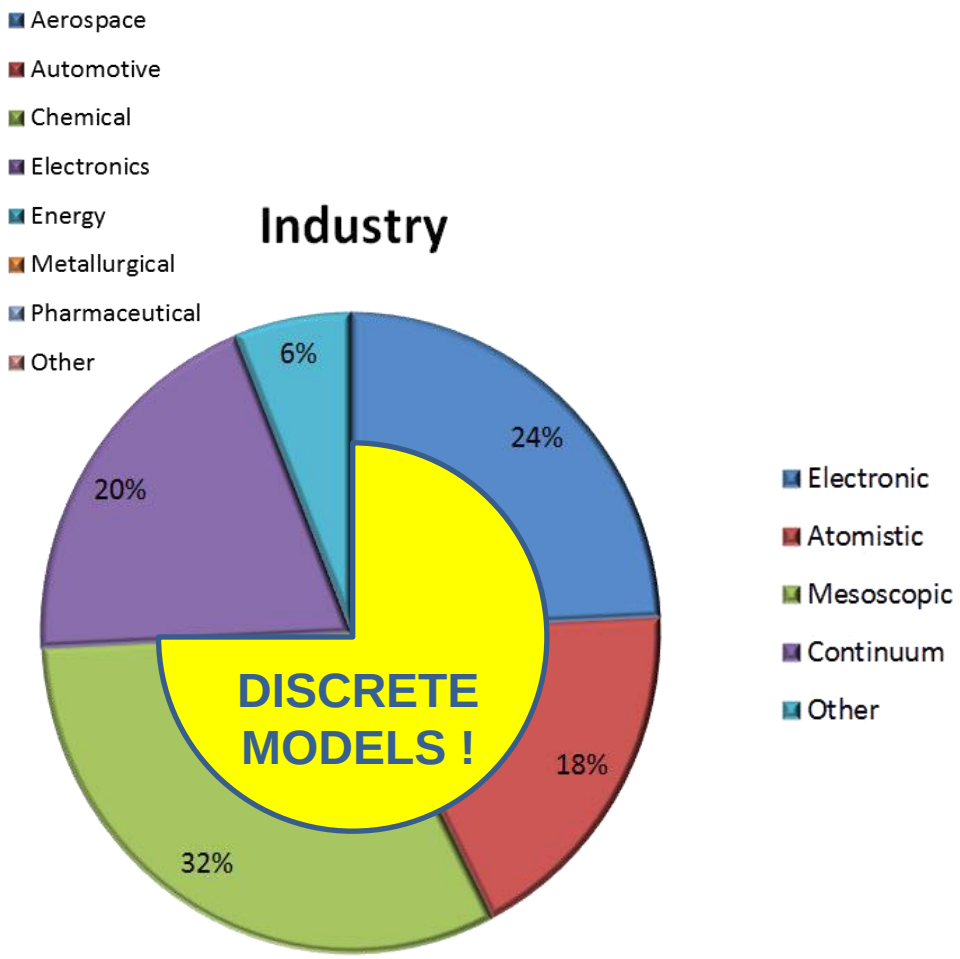
Impact of materials modelling in industrial sector

The impact of materials modelling on the industrial sector is clarified by:

- The increase cost of developing a 21st century product with its prerequisites, requires a smart goal-seeking design procedure where a performance-based (back-engineering) functionality of the product is guaranteed.
- Virtual integration of processes will reduce costs.
- Materials modelling is already part of many business processes but it can become a more impinging part if the economic advantage for the end-user becomes clear.
- Majority of managers (in SMEs) are not aware of importance (and what a difference can be achieved) of a proper material selection and material sourcing to deal with the quality and

Overall analysis of the survey: Applications & models





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Overall analysis of the survey: Applications & models

1 being the most important !	Importance	Urgency	Importance x Urgency
Coupling/Linking	2,13	2,19	4,67
Discrete models	2,21	2,35	5,18
Properties	2,25	2,45	5,51
Industry2020	2,45	2,55	6,25
Accuracy	2,52	2,63	6,62
CSA	2,74	2,80	7,68
IntOp	2,74	2,81	7,71
MMP	3,15	3,21	10,10
BDSS	3,14	3,26	10,26

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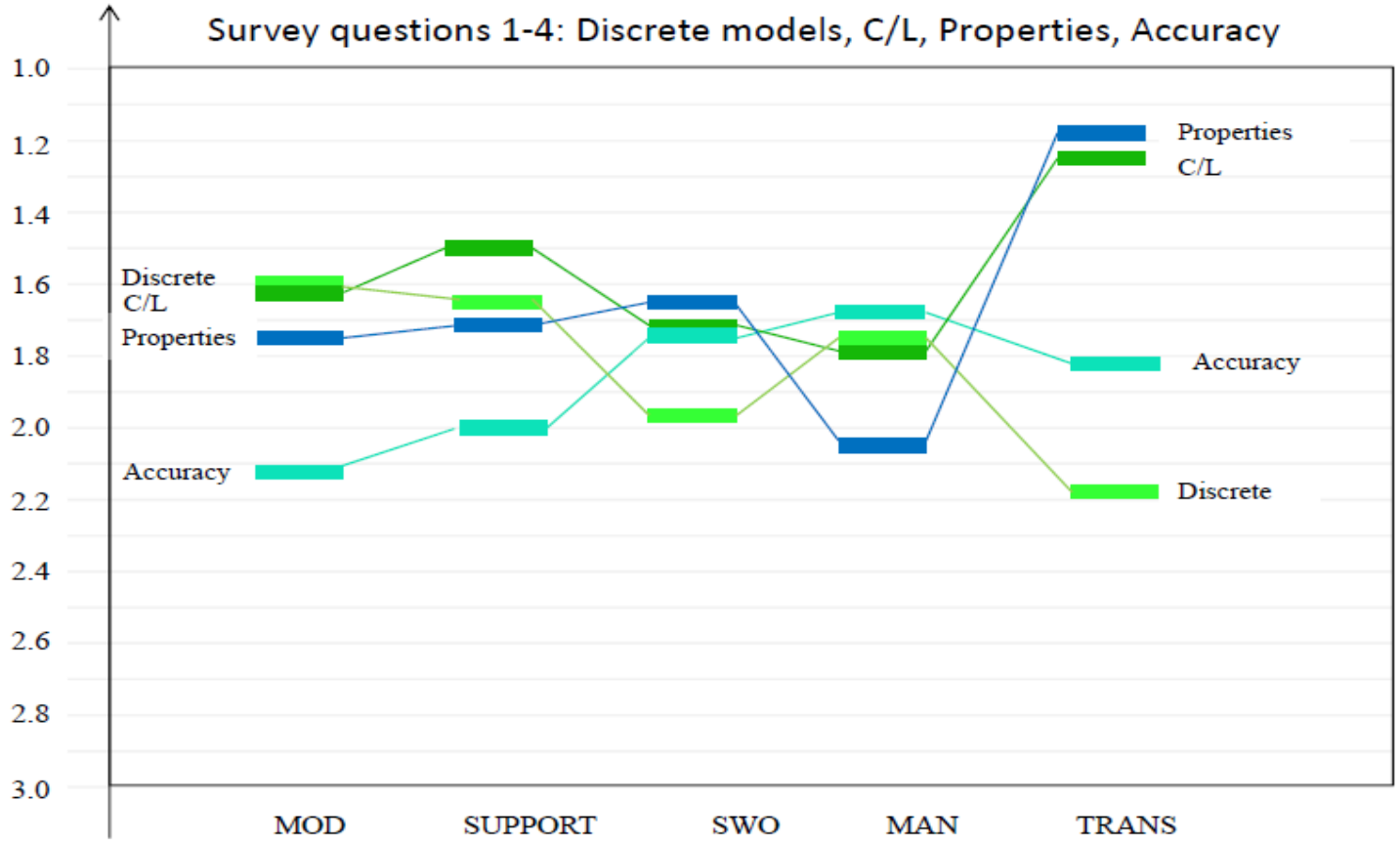
Comparative analysis: Models development



The graphs show the average score for each stakeholder group. Individual answers were in the range 1 - 5 (with 1 highest). The results were exported from the web survey on 5 May 2016. Analysis by KH.

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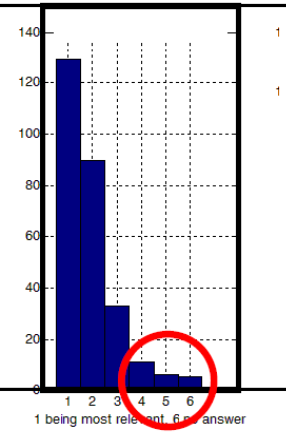
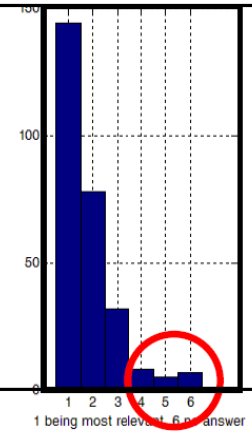
Comparative analysis: Models development

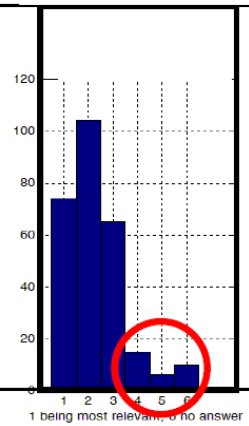
(1) Discrete models



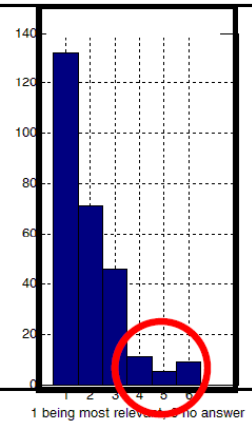
(2) Coupling&Liinking



(4) Accuracy



(3) Properties



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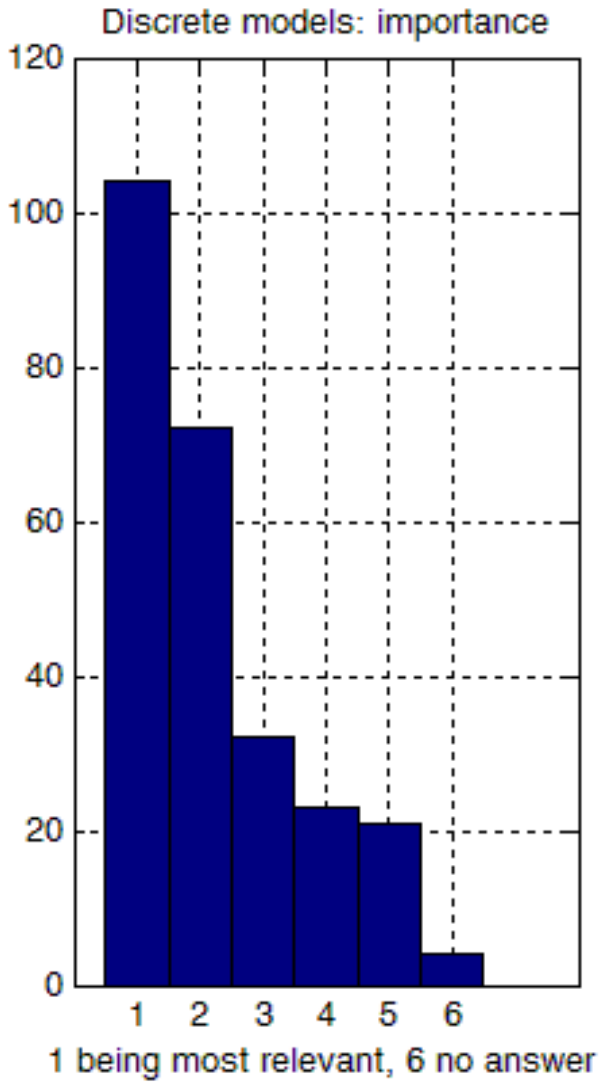
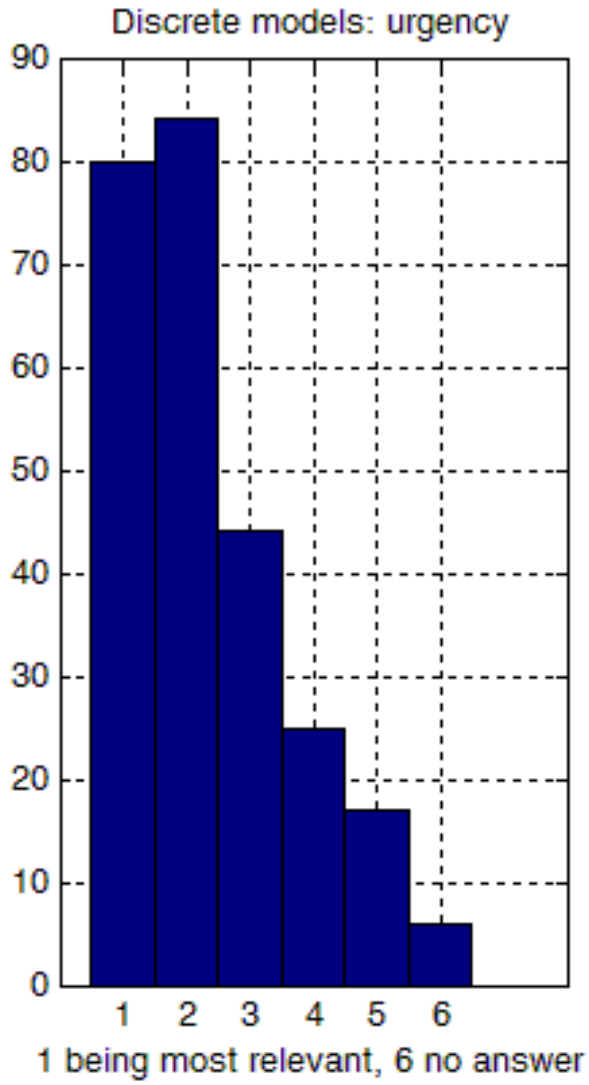
Discrete models (electronic, atomistic, mesoscopic)





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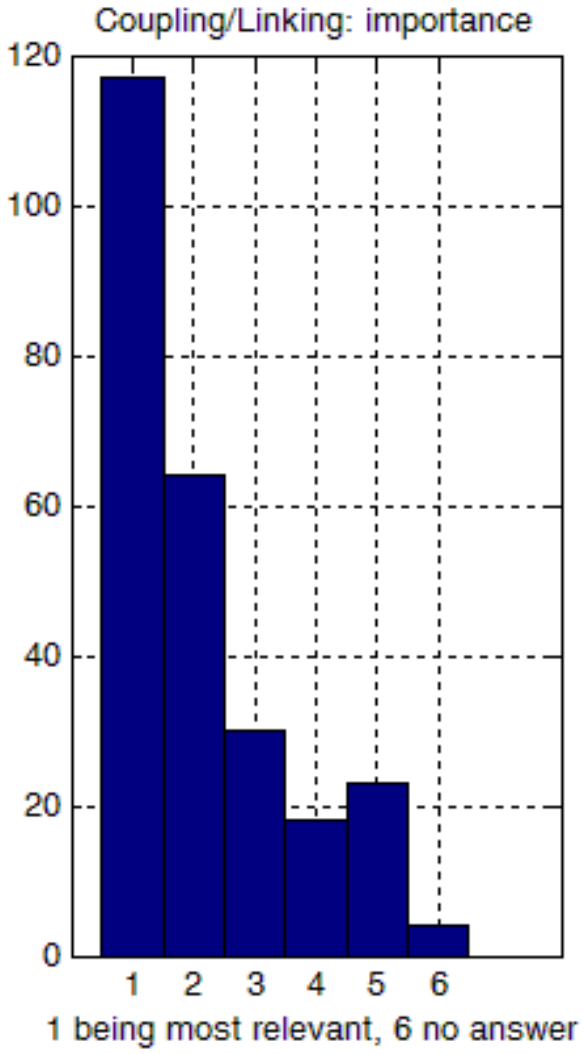
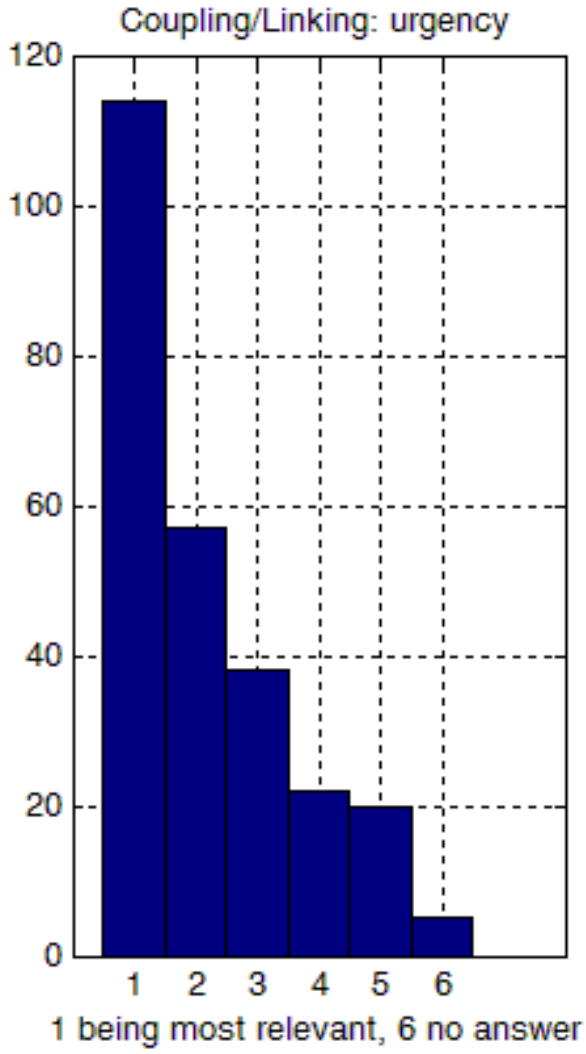
Discrete models (electronic, atomistic, mesoscopic)

- Discrete models received a high priority score among all the stakeholder groups.
- Almost all of the participants in the survey listed one or many fields where the currently available discrete models are insufficient or lacking and hence model development is needed.
- Both predictive and qualitative model needs were mentioned, with a focus on the need for models to handle large and complex systems, such as multi-materials, complex composites and interfaces of different kinds.
- The lack of good atomistic force-fields was mentioned in many answers.
- Strong needs for improvement of workflows were also expressed.

Coupling / Linking





Coupling / Linking

- This topic has a high priority among all stakeholders.
- It is seen as a promising vehicle towards realistic modelling of applications of industrial interest, although the complexity and challenges of the topic are fully recognized.
- Model-wise C/L needs among the discrete models are listed as well as between discrete and continuum models, and between various flavours of continuum models.
- Both top-down and bottom-up approaches for materials design, property calculations and process simulations are mentioned.
- Here not only challenges in terms of the model-focussed efforts, i.e. the strategies to select what degrees of freedom to dispose of (or add) in the coupling and linking process, are highlighted in the comments.

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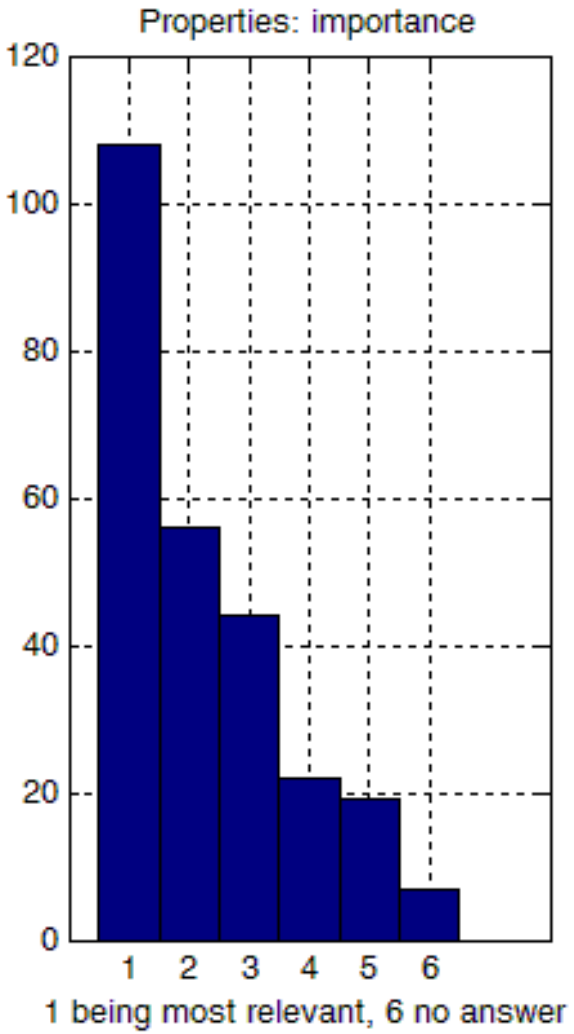
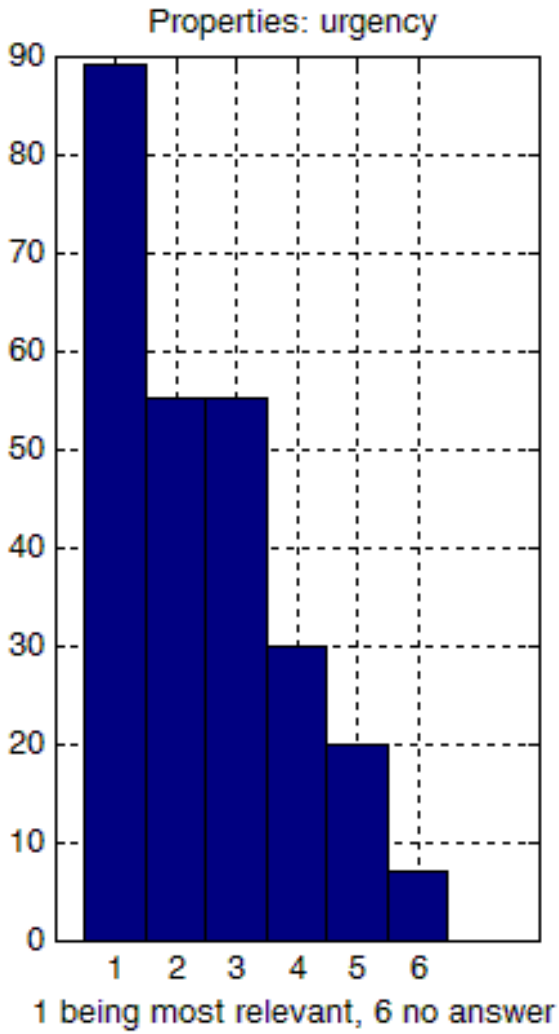
Extracting materials properties





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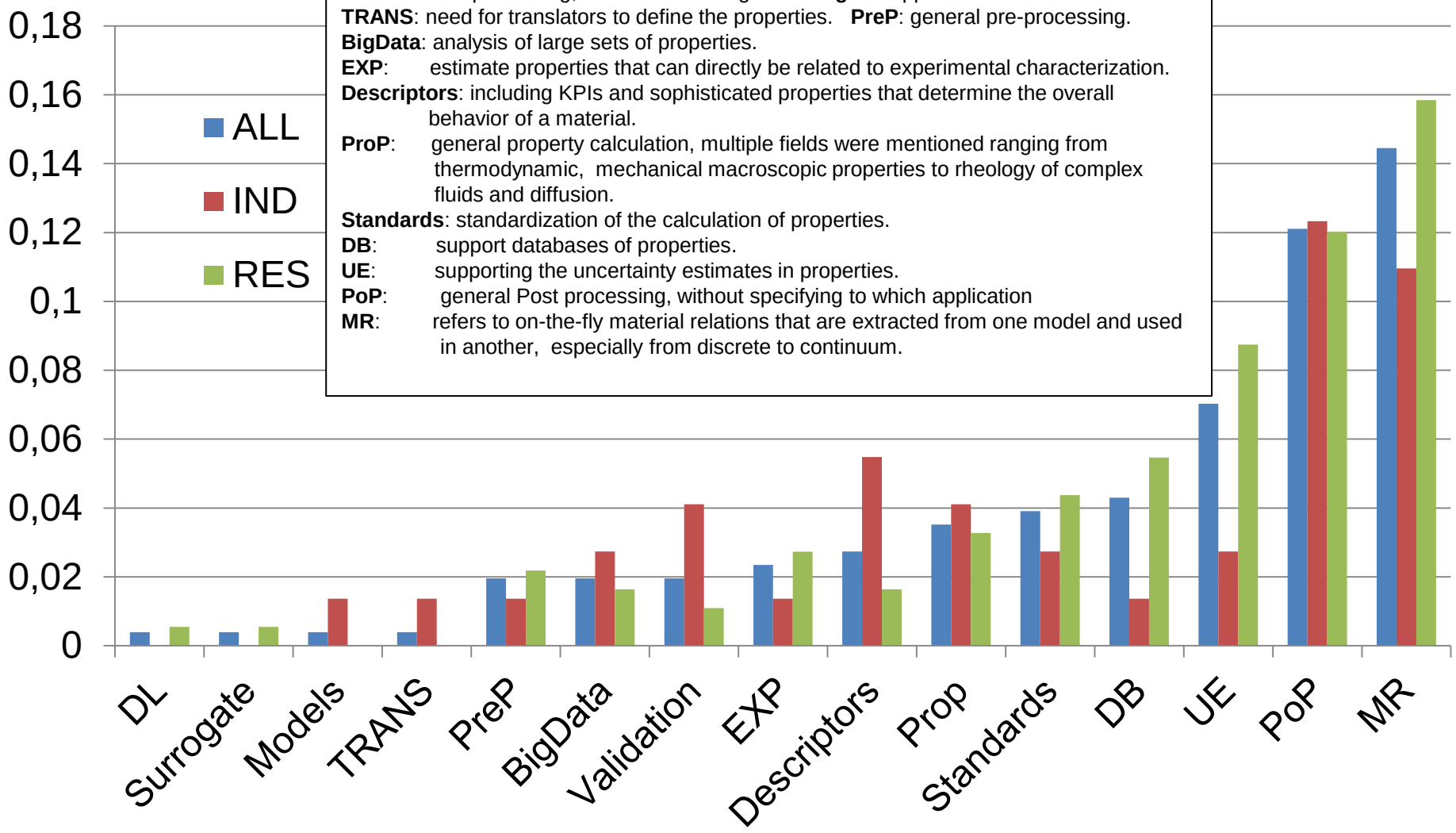
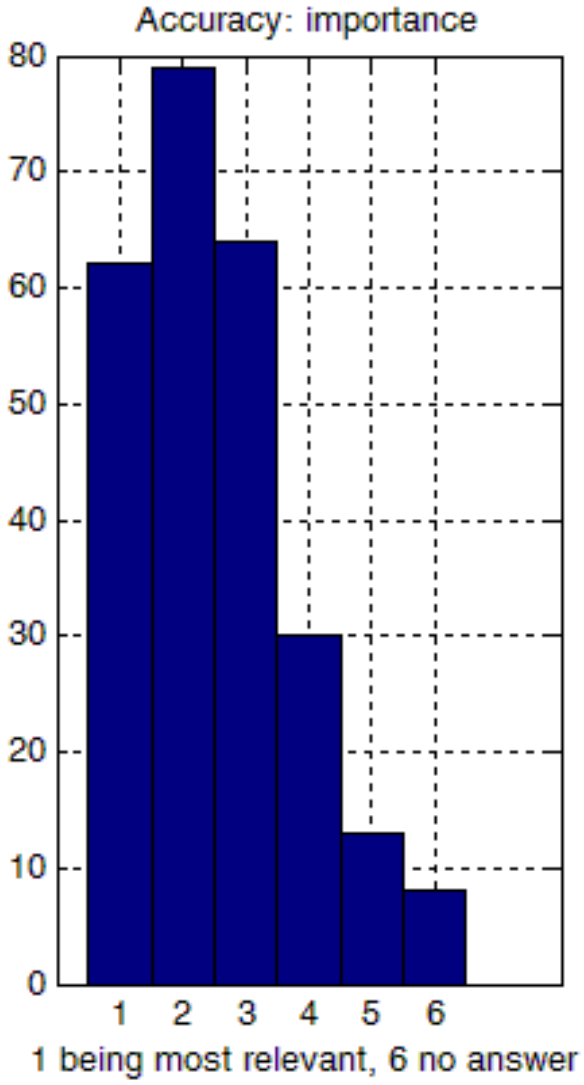
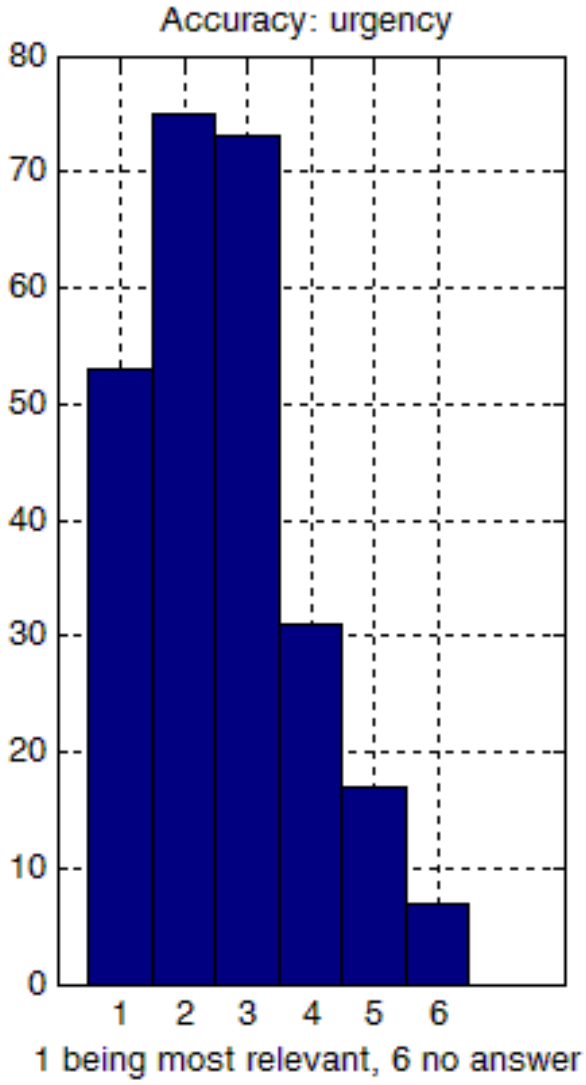
Extracting materials properties

DL: Deep Learning, Machine Learning. **Surrogate**: approximate models.
TRANS: need for translators to define the properties. **PreP**: general pre-processing.
BigData: analysis of large sets of properties.
EXP: estimate properties that can directly be related to experimental characterization.
Descriptors: including KPIs and sophisticated properties that determine the overall behavior of a material.
ProP: general property calculation, multiple fields were mentioned ranging from thermodynamic, mechanical macroscopic properties to rheology of complex fluids and diffusion.
Standards: standardization of the calculation of properties.
DB: support databases of properties.
UE: supporting the uncertainty estimates in properties.
PoP: general Post processing, without specifying to which application
MR: refers to on-the-fly material relations that are extracted from one model and used in another, especially from discrete to continuum.



Extracting the accuracy





Extracting the accuracy

- A majority of the responses comments state that this topic represents an important and even crucial area.
- It is also clear from the answers that model assessment and error quantification exposes many facets. Achieving a reliable direction, a qualitative trend, may be the key point.
- Thus among the manufacturers, several expressed that reliable qualitative trends derived from modelling are useful, while predictive quantitative data may be the ultimate goal.
- It was pointed out by many respondents that accuracy can be an ill-defined concept, as one and the same model can be either accurate or unprecise depending on how it is applied. Here the remedy can lie in the inclusion of more of the relevant physics contents for the application at hand.

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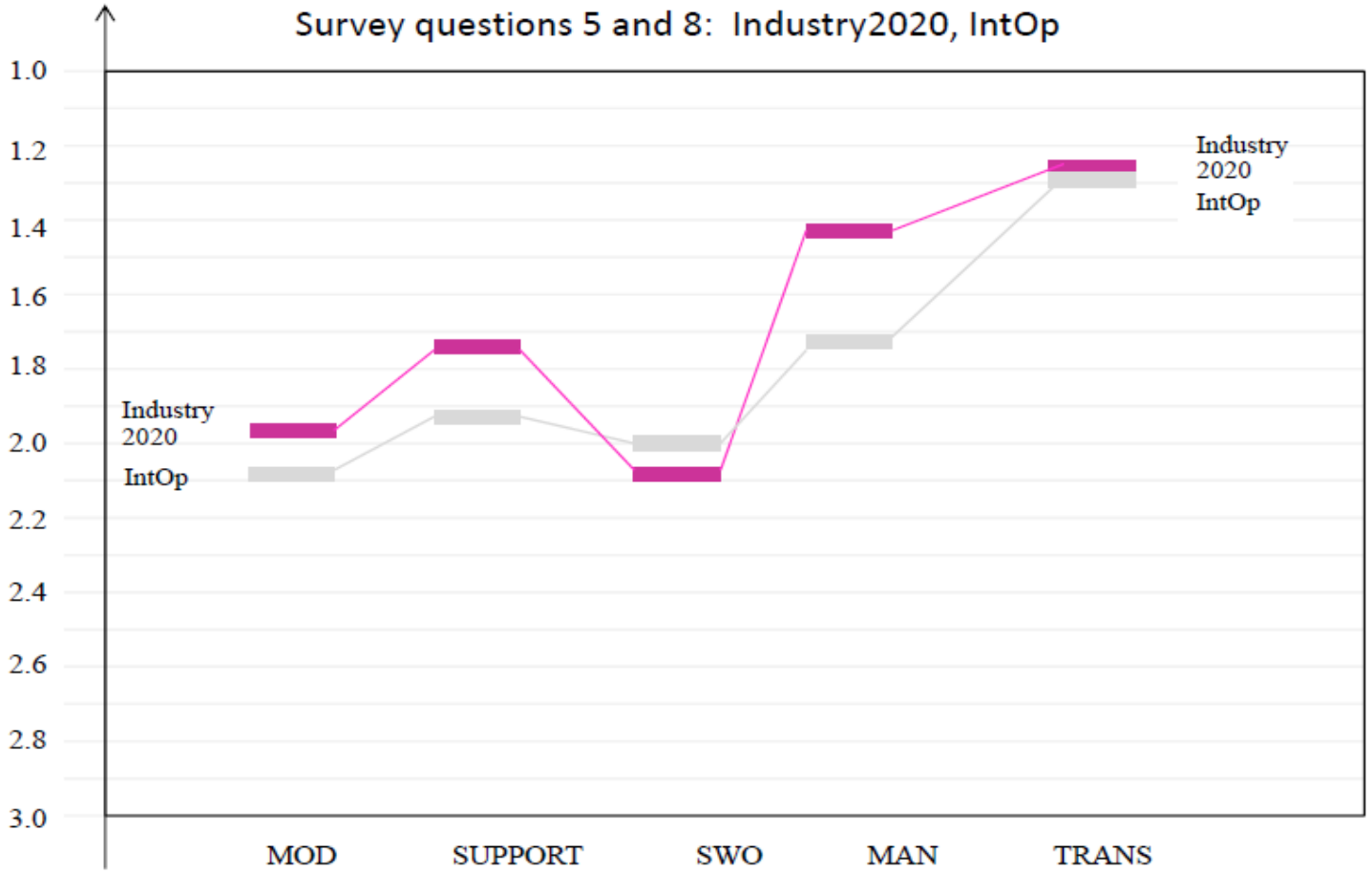
Comparative analysis: Industry2020 & IntOp



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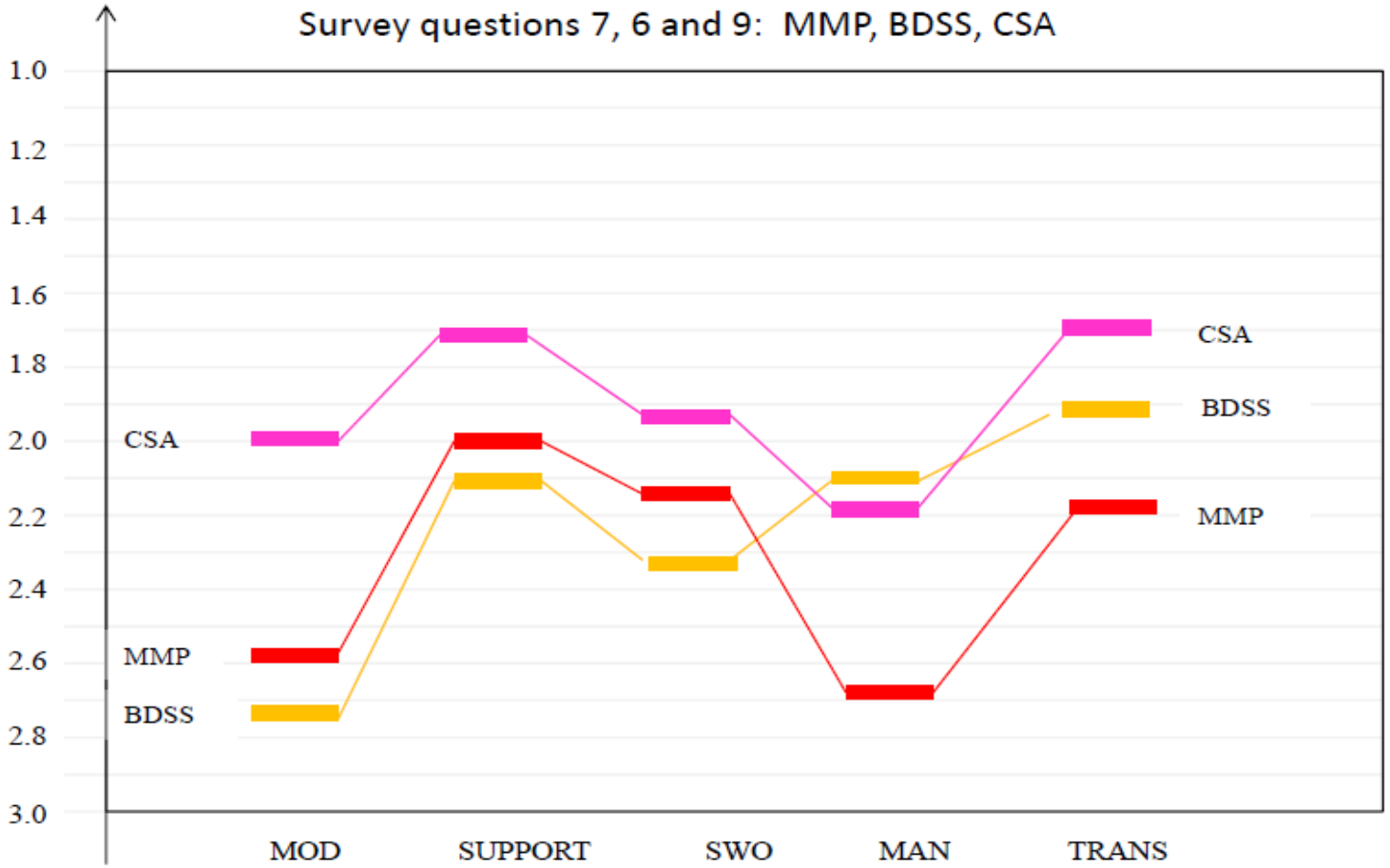
Comparative analysis: MMP, BDSS, CSA



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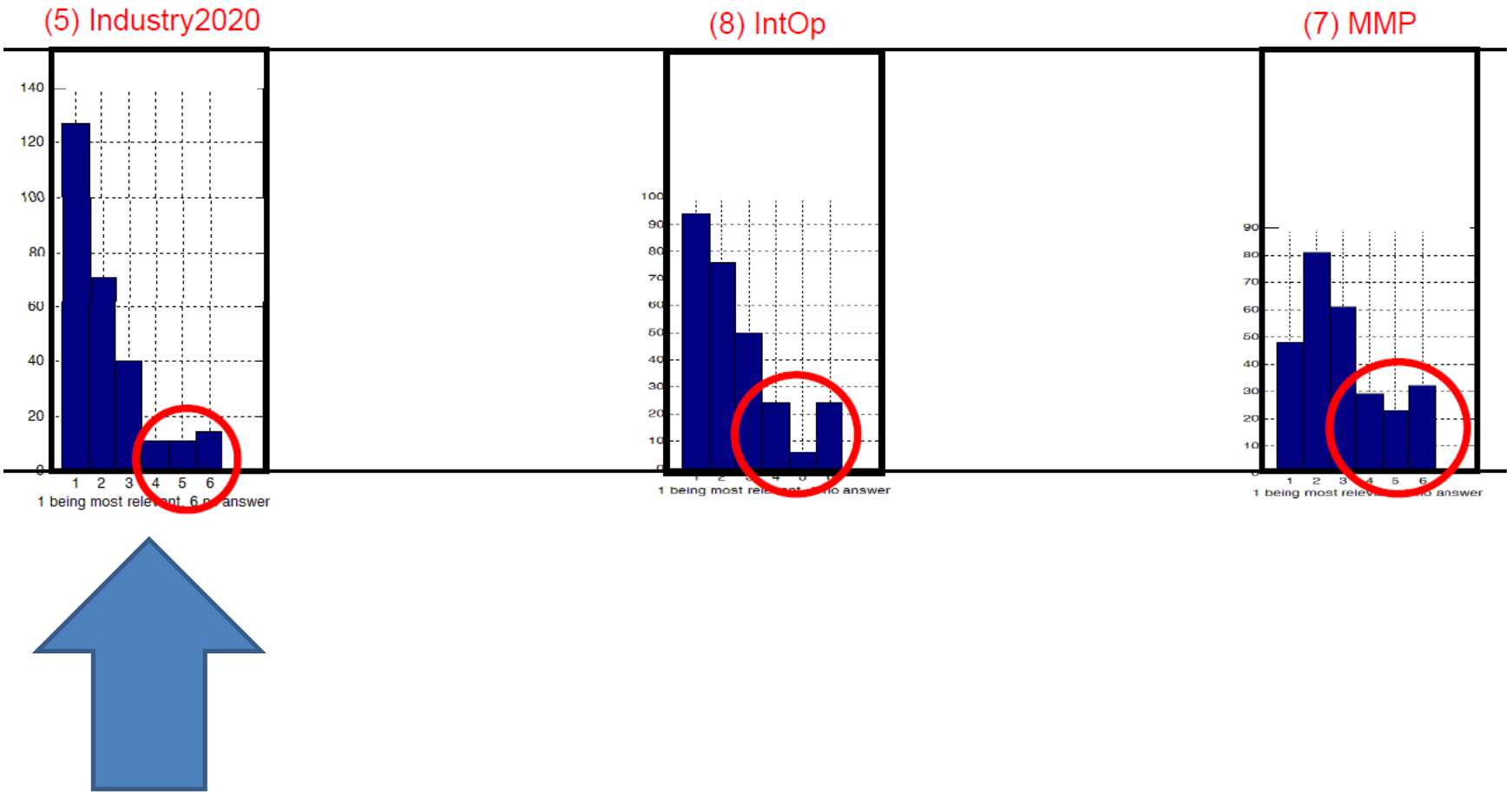
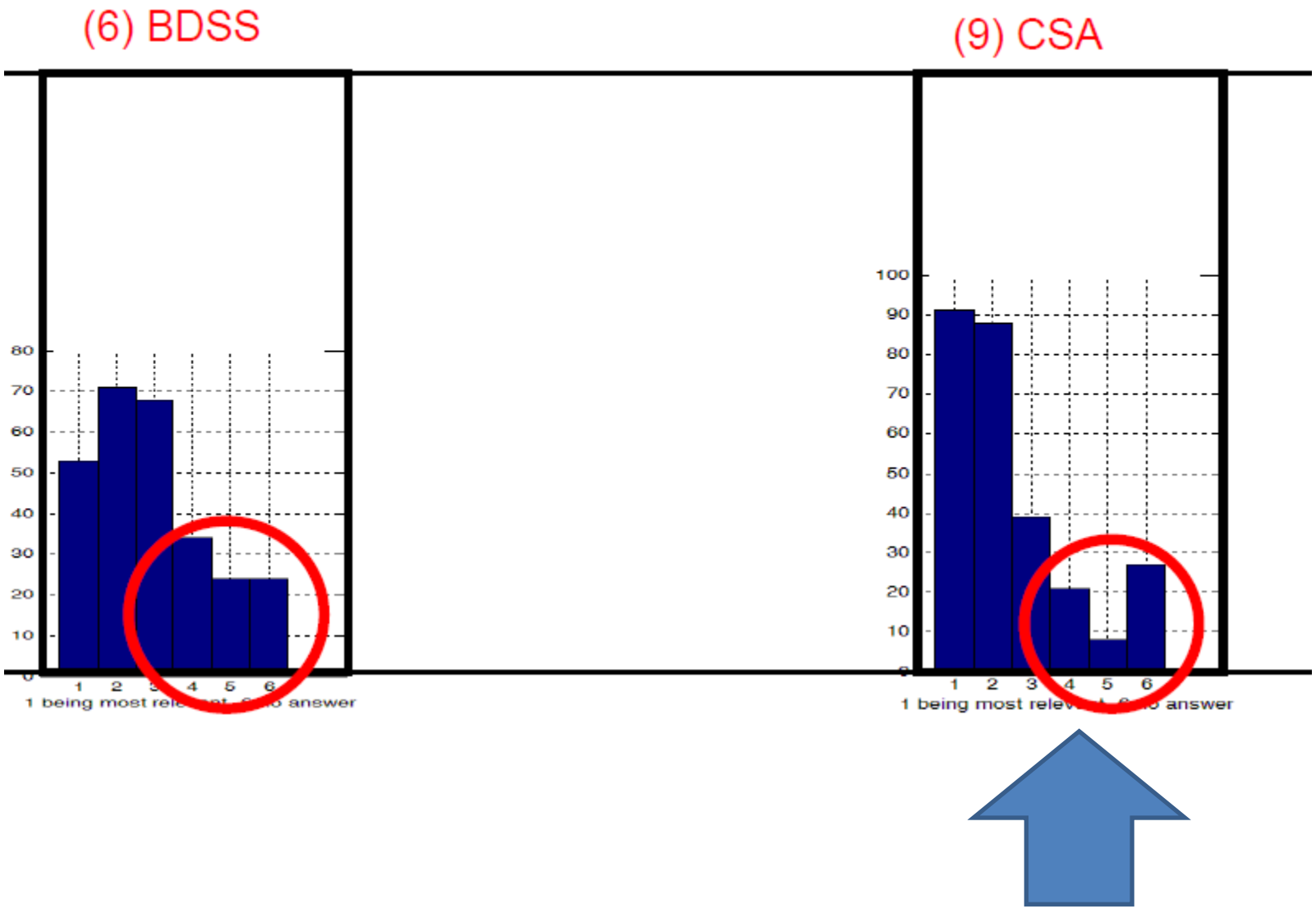
Comparative analysis: Industry2020, IntOp & MMP



Comparative analysis: BDSS & CSA



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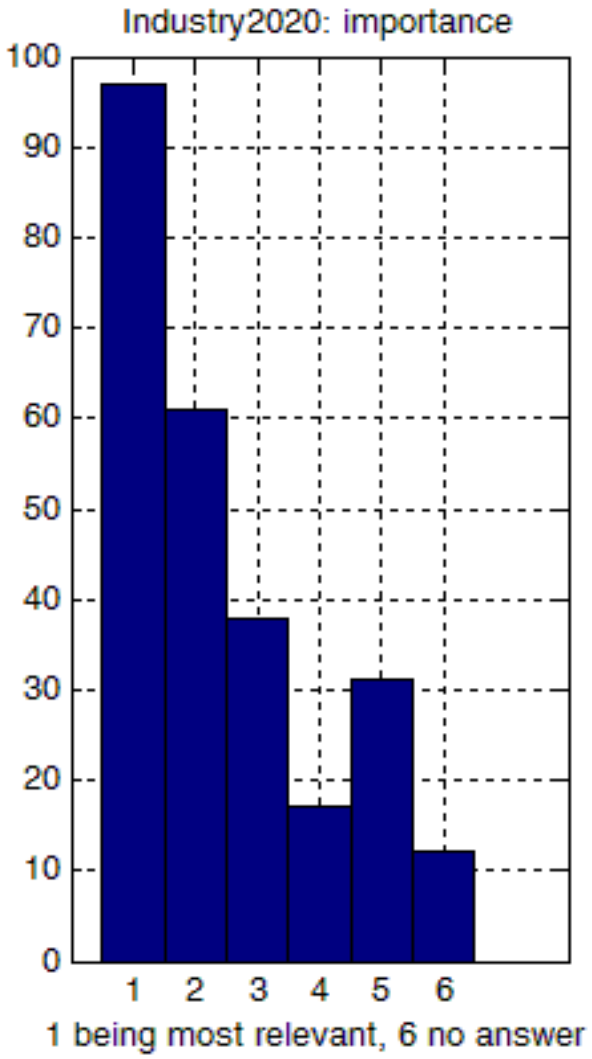
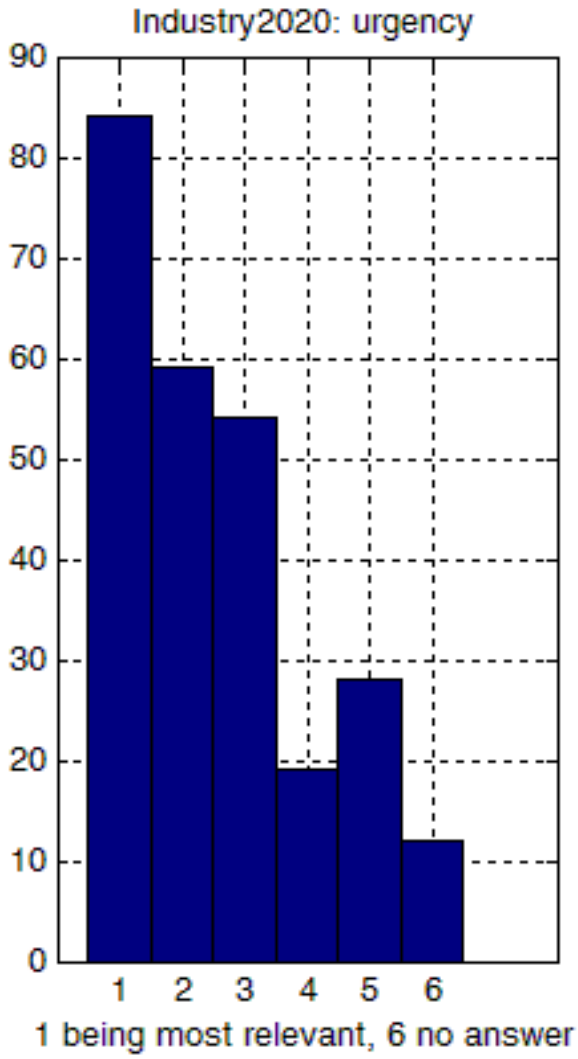
Models in manufacturing & processing (Industry2020)





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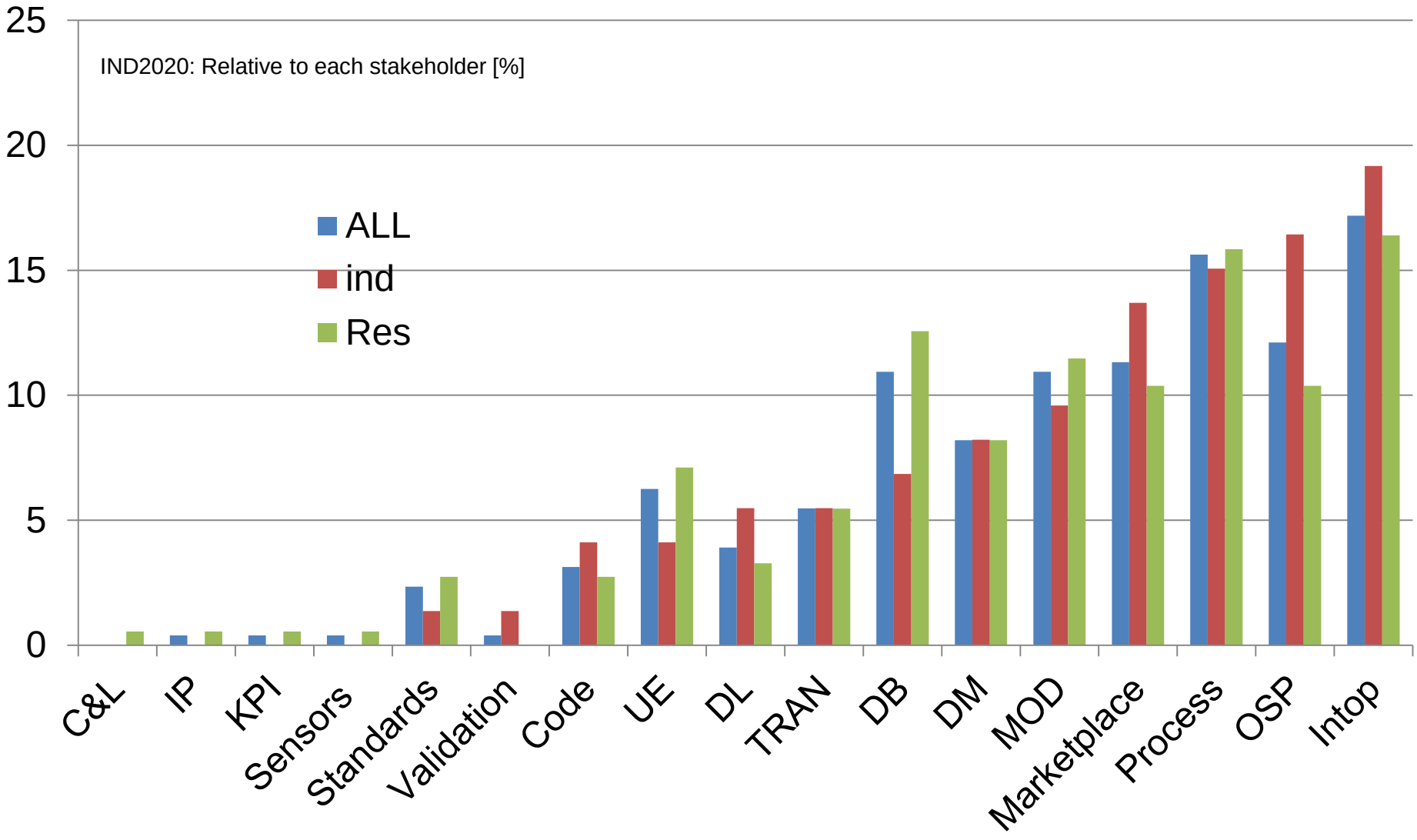
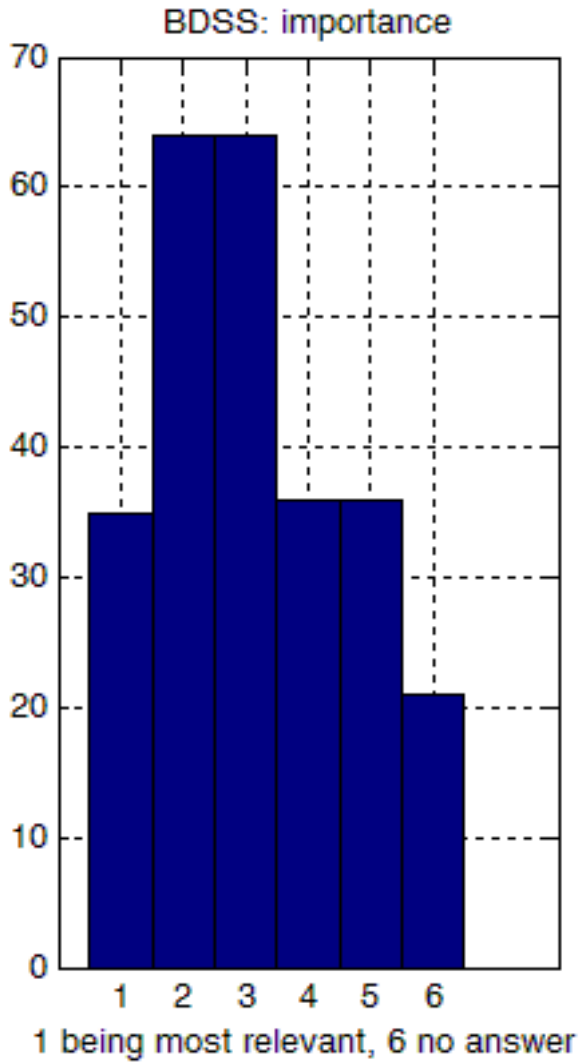
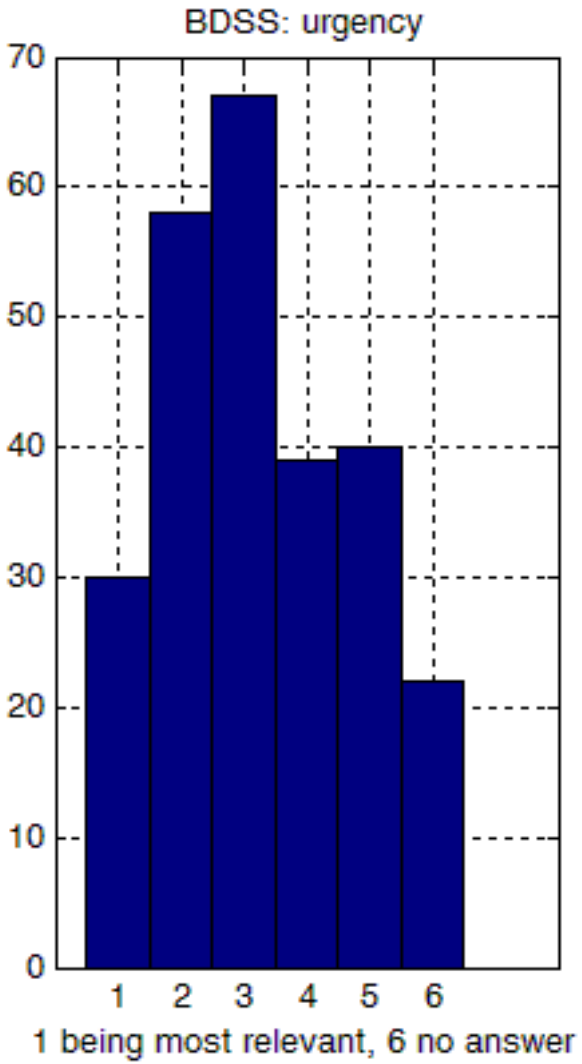


Business Decision Support System (BDSS)





Business Decision Support System (BDSS)

- Impacts to be expected:
  - Upscaling and market introduction with increased speed and reduced risk;
  - Virtual integration of processes will reduce costs;
  - Minimize expenses and time needed in achieving a functional and marketable end product;
  - Suggest direction of new material development.
- Estimation and quantification of impact
  - Financial data and multi objective optimisation toolboxes;
  - Indicators for evaluating the impact.
- Challenges and requirements
  - Robust semantic interoperability schemes;
  - Novel artificial intelligence models;
  - A more smart computationally oriented technique is required.

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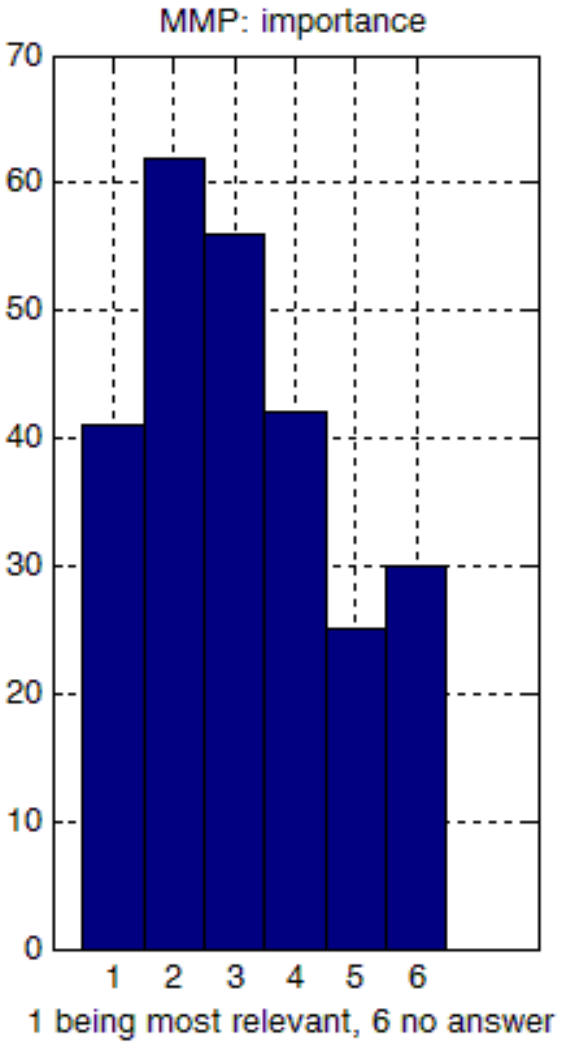
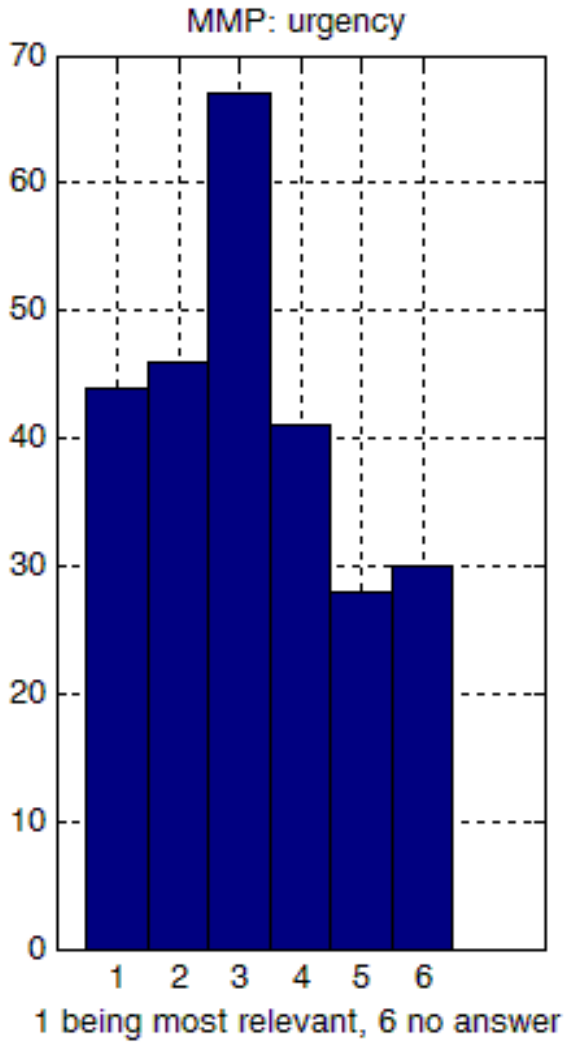
Modelling market place and dataspaces





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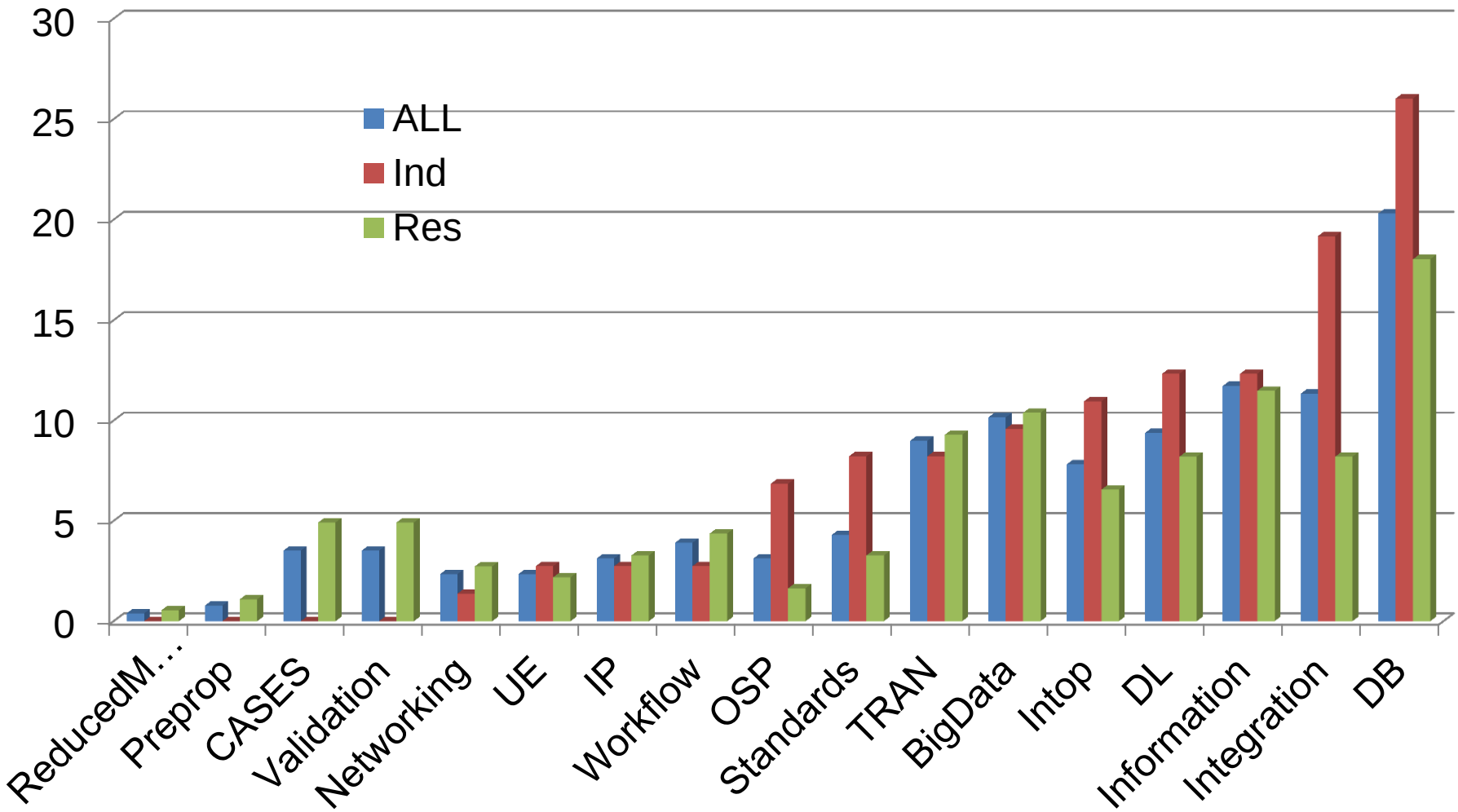
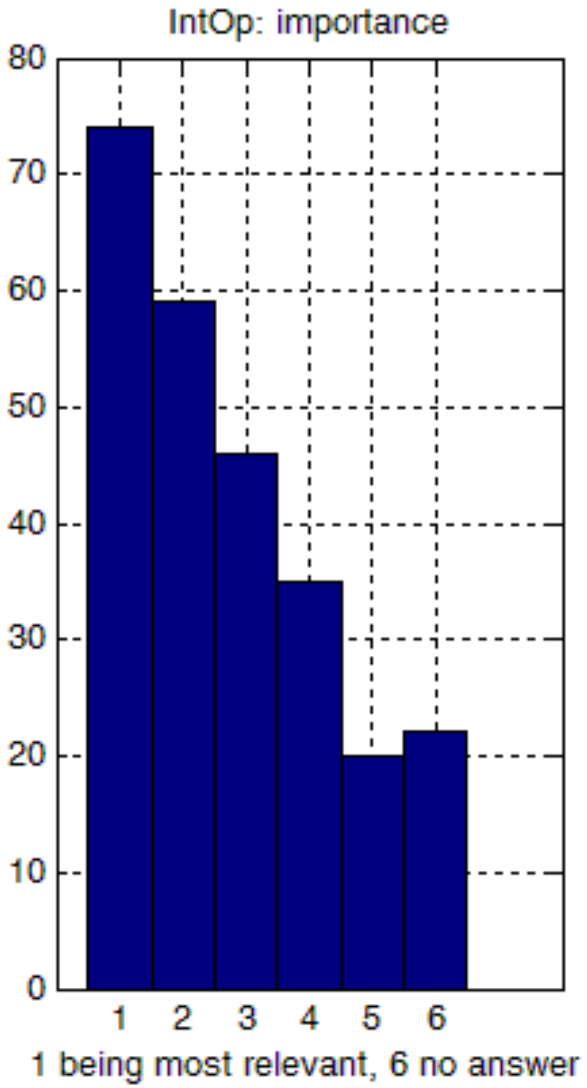
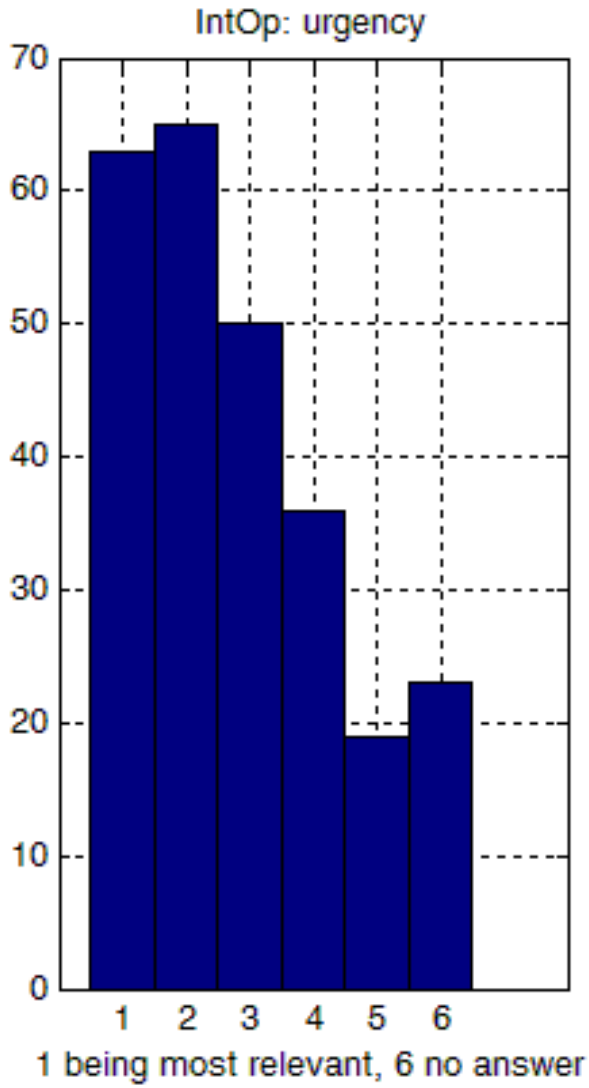
Modelling market place and dataspaces



Integrated workflows and interoperability





Integrated workflows and interoperability

- Semantic interoperability in materials modelling.
- The big challenge is to combine models not designed to communicate with other in a useful way. This requires robust semantic interoperability schemes.
- Businesses require the lowest cost for a specific purpose. The choice of material is part of that and better decision support systems for materials are needed.

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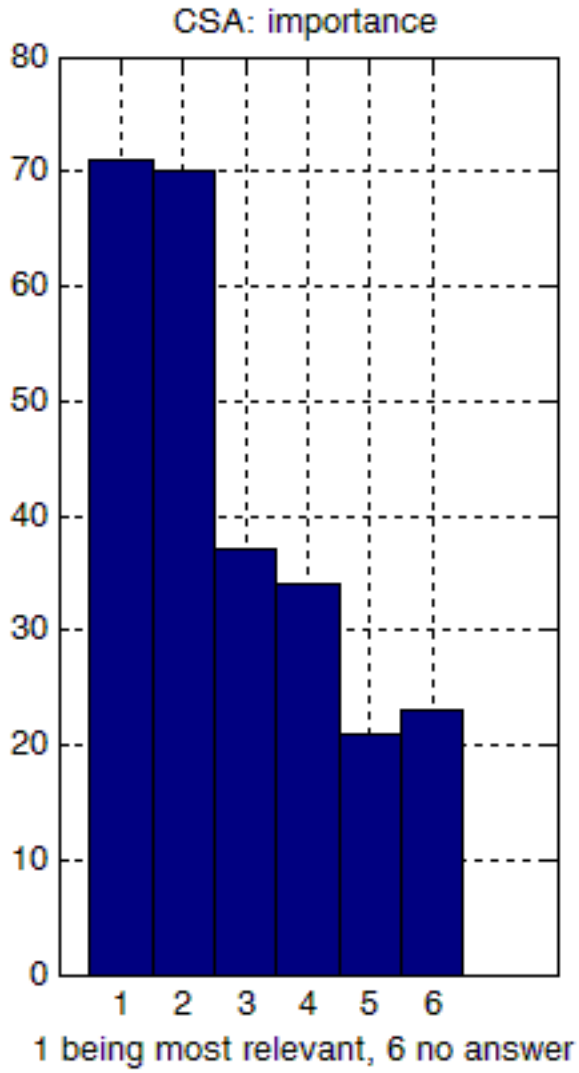
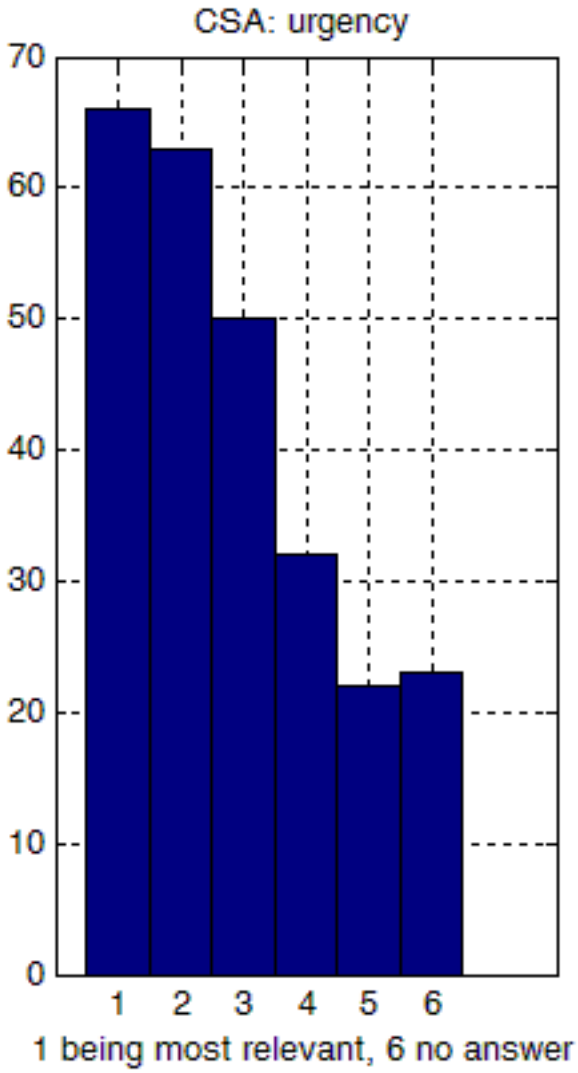
Coordinating network





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Coordinating network

- Continuation of the EMMC CSA is important.
- Enhance the networking and communication between all existing modelling communities, with more links to industrial materials producers.
- Not only transfer the knowledge from academic to industry but also vice-versa: a clearly defined need of models coming from industry.
- It is important to show stories of success. This requires support to develop multiscale models for industrial applications.
- Provide and start from simple solutions/cases and killer applications that manufacturers will feel as a real gain and benefit.

Summarizing…

- The nine topics, which emerged from the EMMC working groups, all received a positive response from the participants of the survey.
- This is particularly clear for the use of discrete models and the development of more effective coupling and linking workflows.
- It is very clear that the lack of adequate models is the main bottleneck for modelling industrial problems.
- The most relevant topics will be refined by including the comments collected by the survey, in order to clarify better
  - (a) the challenge,
  - (b) the industrial impact (already reported in many replies by industrial stakeholders),
  - (c) the scope and the most appropriate action.

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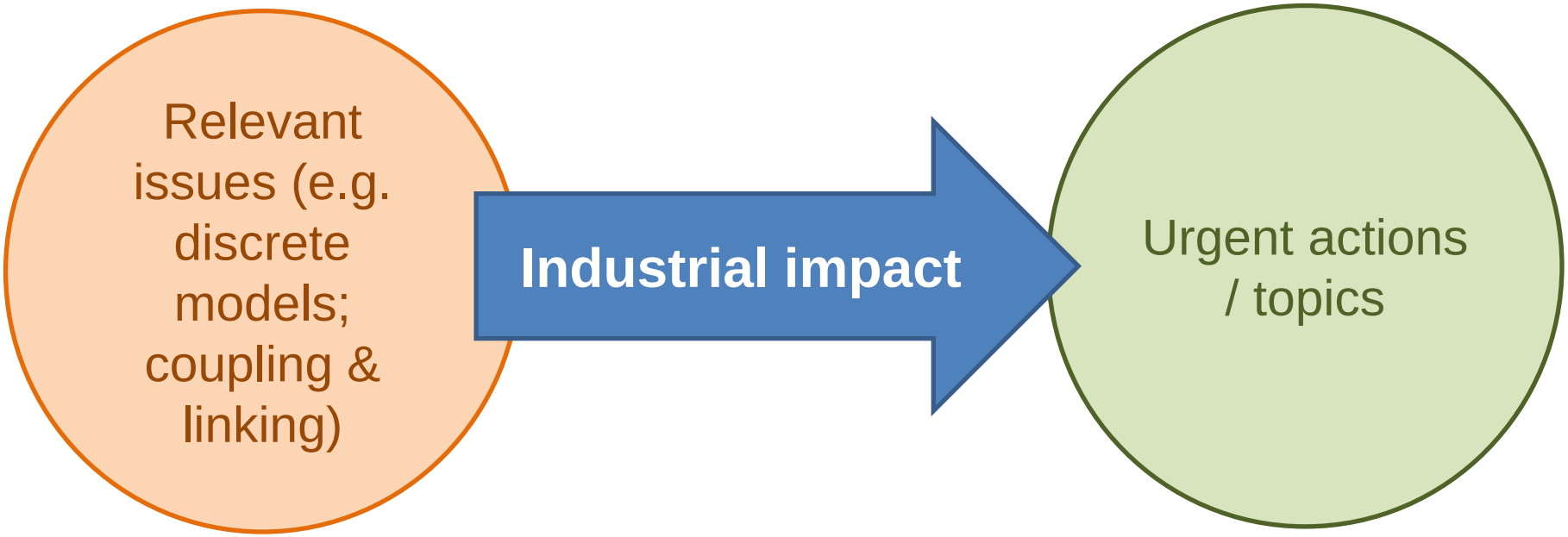
From relevant issues to urgent action / topics



URGENT ACTION: Going down and safely back up

- Relevance for European Industry: Accurate selection of structural materials with desired KPIs for new products requires top-down design, which implies exploring more detailed structures (going down) and then homogenize their properties (going back up). Unfortunately there is a lack of systematic models and workflows for generating relevant detailed structures and for computing from them KPIs.
- Specific Challenge: To develop a systematic procedure for sampling the detailed structures, preserving the most relevant physics/chemistry at each step and preserving the required accuracy for industrial KPIs.
- Expected Impact: Time saving, predictable and trackable simulation workflows, best-possible detailed insight.
- TRL: from 4 to 6; Type of Action: RIA

URGENT ACTION: Discrete models

- Relevance for European Industry: 75% of the manufacturing industries use discrete (e/a/m) models for their products. However currently available discrete models are insufficient or lacking and hence model development is needed.
- Specific Challenge: To develop industrially-oriented models to handle large and complex systems, such as multi-materials, complex composites and interfaces. In particular, discrete models require systematic atomistic force-fields and improved workflows.
- Expected Impact: Materials insight in upscaling and market introduction of new products; Minimize expenses and time needed in achieving new products; Suggest direction of new material development.
- TRL: from 4 to 6; Type of Action: RIA


thank you
danke
merci
gracias
obrigado
dziękuję
bedankt
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謝謝
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