EMMC Translation Workshop

TRAINING ACTIVITIES AND MODEL GAPS

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Outline

- Training activities:
  - Economic impact of modeling and translation training
  - Business Decision Support System (BDSS) & Marketplaces for training
  - More specifically on test cases:
    - Translation test case 1: long-term partnership example
    - Translation test case 2: neutrality example
- Update on model gaps

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Generic/universal Translation steps

1) **Good understanding of the business case**

2) **Good understanding of the industrial case**

3) **Analysis of the experimental data available within the client:**

4) **Translation to (preferably more than one) modelling workflows**

5) **Propose to the client modelling executor(s) and strategy for model validation**

6) **Translation of the modelling results to information that is understandable, reliable and usable by the client**

TRAINING

Economic training and its impact

TRAINING

TECHNICAL

input data
modelling solutions
simulation strategies
computational effort
accuracy & error
expected outcome
…

ECONOMICAL

cost assessment
resource investment
return on investment
risk assessment
decision making
…

TECHNICAL ACADEMY

OK

ECONOMICAL ACADEMY?

EC expert? Prof. of economics?

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Translation training: overview

Economical aspects

- balance between investments (resources and expertise) and expected return
- economic background to advice on costs and time to solution
-human factors: skills, readiness, management of subcontractors

Technical aspects

- four different materials models (electronic, atomistic, mesoscopic and continuum)
- accuracy of modelling efforts
- input of data from the industrial stakeholder ←→ workflow/ simulation tools
- confidentiality issues of industrial data
-expertise for results interpreta-tion

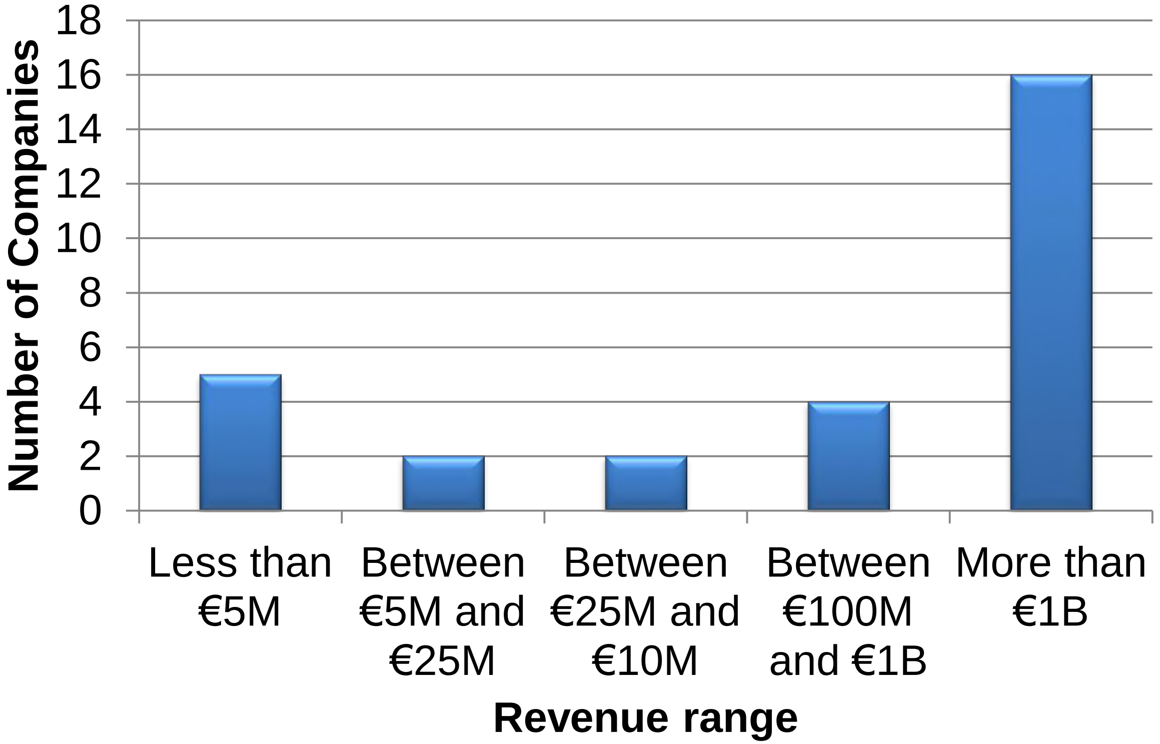
Neutrality

- give neutral advice; third parties might be involved in the implementation of the modelling workflow
- be free from hidden self-interests: must place the interest of the clients before the interests of the Translator
- more than one solution should be proposed
- proposed solution should not be biased towards the Translators favourite models, methods or software tools

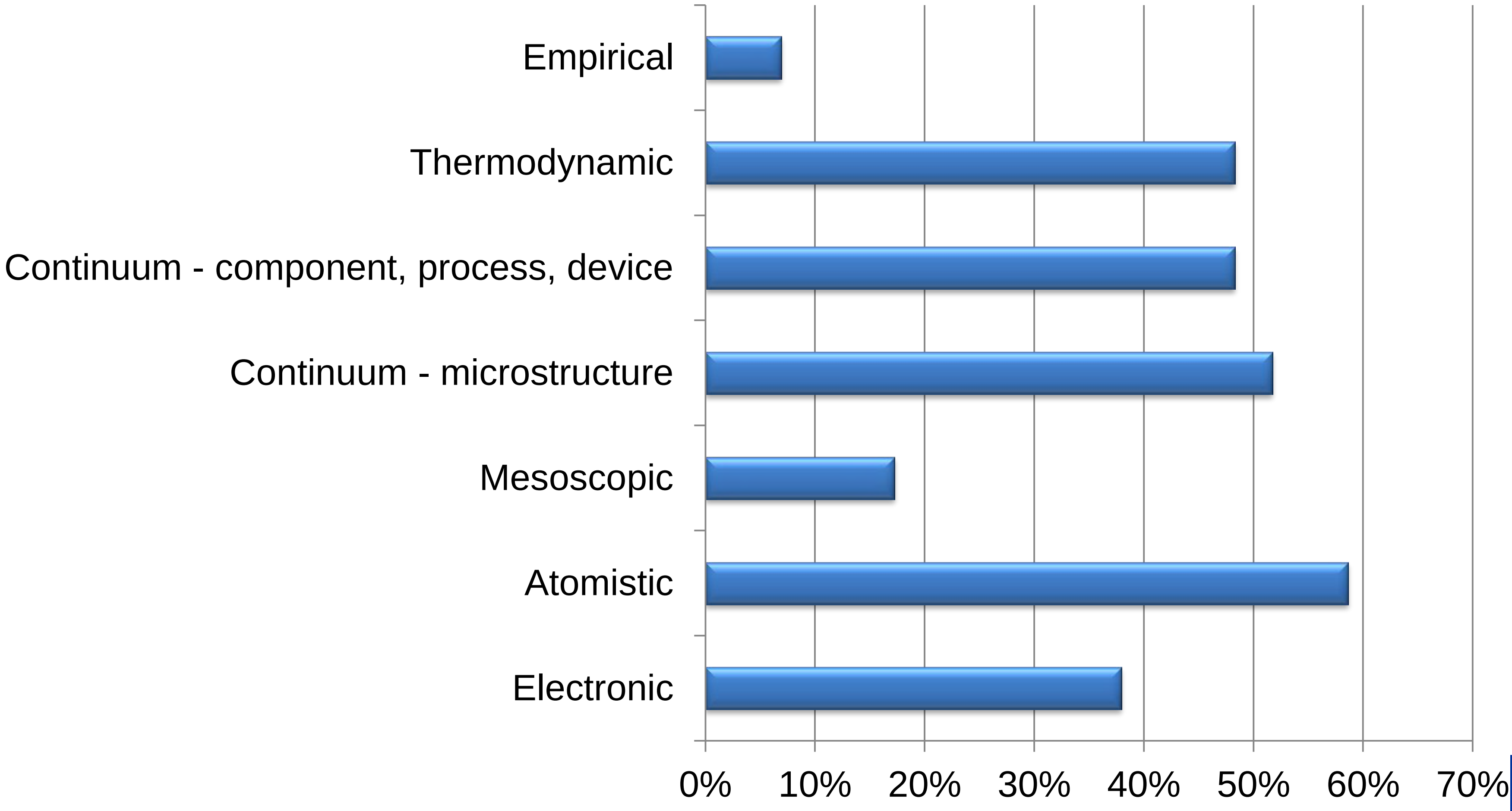
TRAINING

EMMC - Economic impact survey 2015

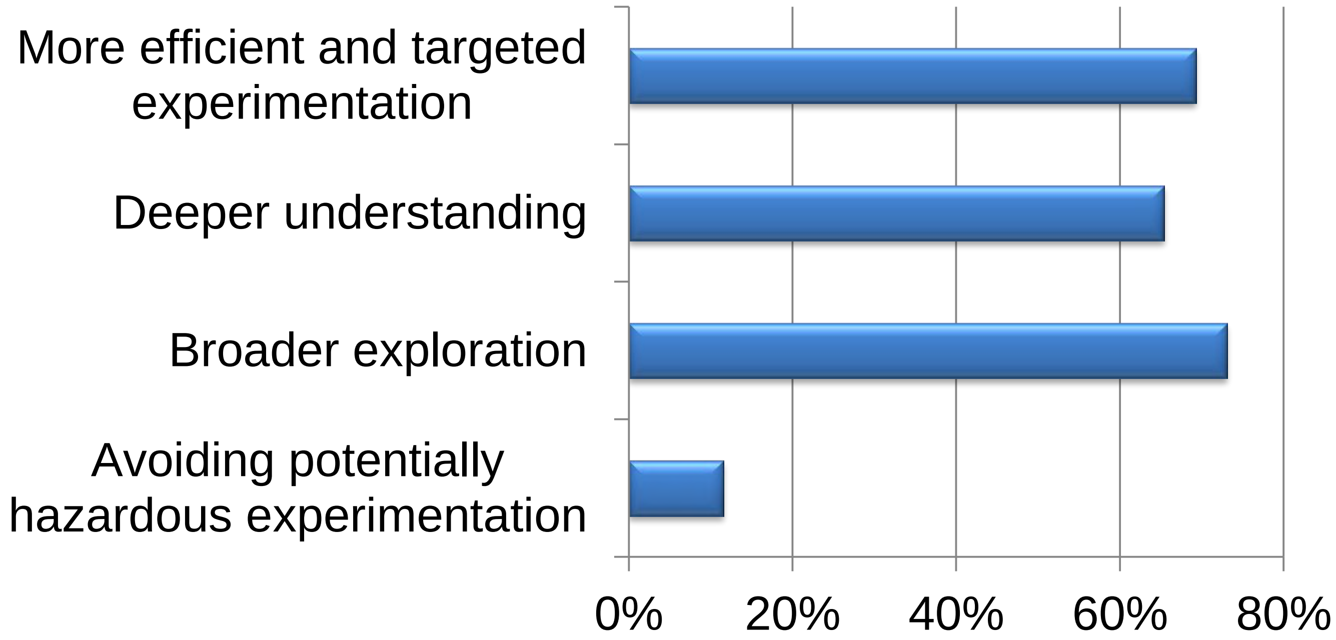
- 150 manufacturing organisations invited; 34 responses (23%).
- 5 responses from companies that have been involved in materials modelling projects but do not carry out materials modelling
- **29 responses used for further analysis.**



Types of materials modelling used



R&D process improvements



Return-on-investment (ROI) models:

cost-benefit analysis requires much more detail and <u>knowledge</u>…

Business Decision Support System (BDSS)

Business decision support system (BDSS)

- **COMPOSELECTOR "*Multi-scale Composite Material Selection Platform with a Seamless Integration of Material Models and Multidisciplinary Design Framework*"**
- **FORCE**

The EMMC will coordinate all H2020 BDSS !

Let us consider COMPOSELECTOR as a case study…

Business Process Model and Notation (BPMN)

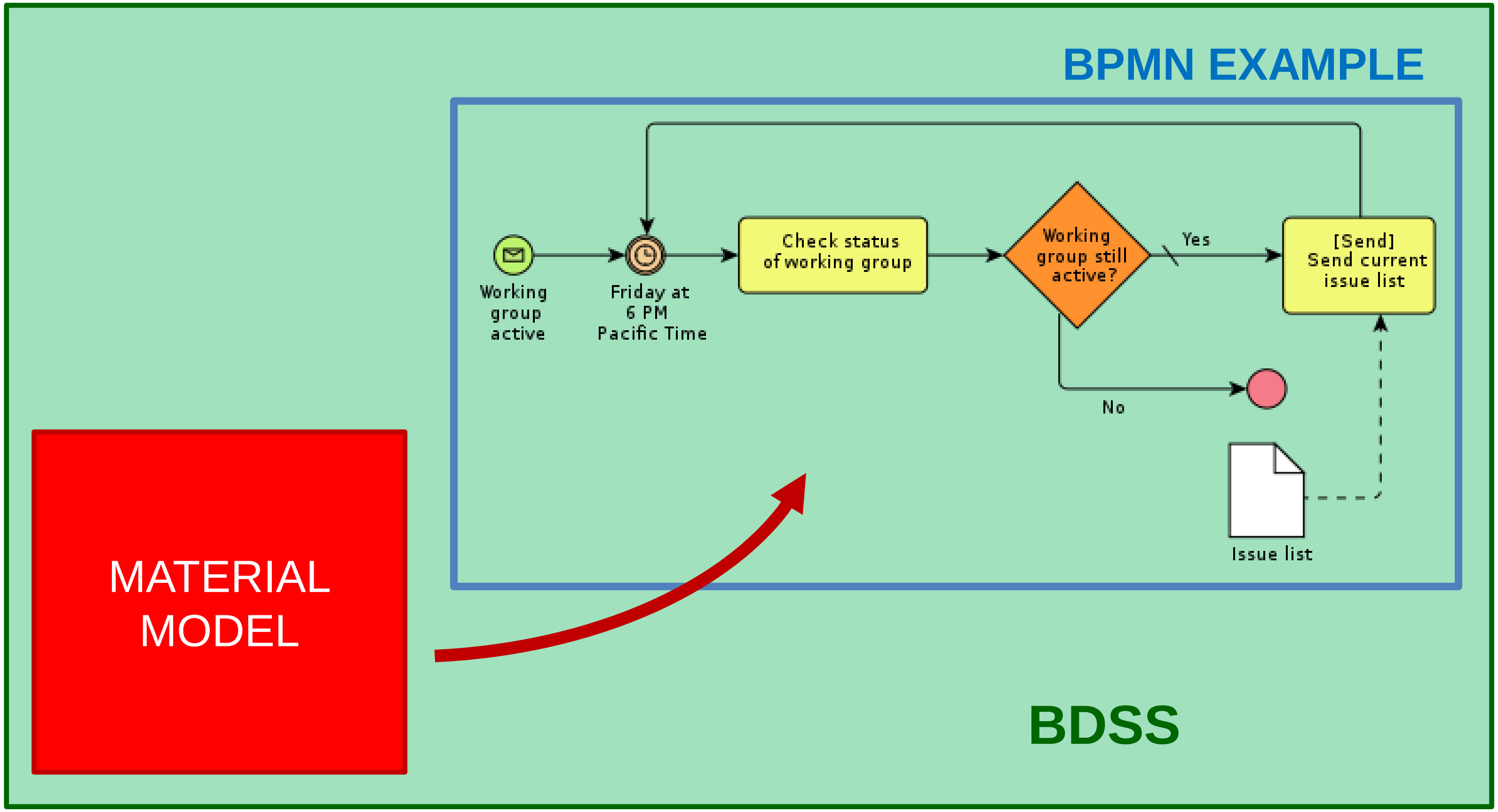
The **Business Process Model and Notation** (BPMN) is a graphical representation for specifying business processes in a business process model.

ISO/IEC 19510:2013

New and more complete models, including more information, e.g. **Business Decision Support Systems (BDSS)** are currently under development…

Let us see how it works

BPMN + MATERIAL MODELs = BDSS (for materials selection)



BDSS issues

- In BDSS: - define modelling capabilities (by MODA) as soon as possible, with also possible interoperable alternatives; - specify for each MODA solver the costs, namely workforce, training, software and hardware costs = modelling cost; - specify for each MODA solver the expected accuracy

- The modelling ROI comes from evaluating different modelling scenario, including accuracy, (see above) into the BDSS, namely the current economical decision process. Example: substitute one experimental material characterization by one modelling procedure. The cost difference between current practice and modelling one = modelling ROI

Marketplaces for training

Online marketplaces for training activities

MARKETPLACES

- **VIMMP "Virtual Materials Market Place"**
- **MARKETPLACE**
- **EMMC modelling marketplace (EMMC MMP):** under construction

The EMMC MMP will coordinate all H2020 market places !

- **NanoHub (USA):** up and running from several years (since 2002)

Here we present NanoHub as one of the possible ways to handle a marketplace for training activities and more…

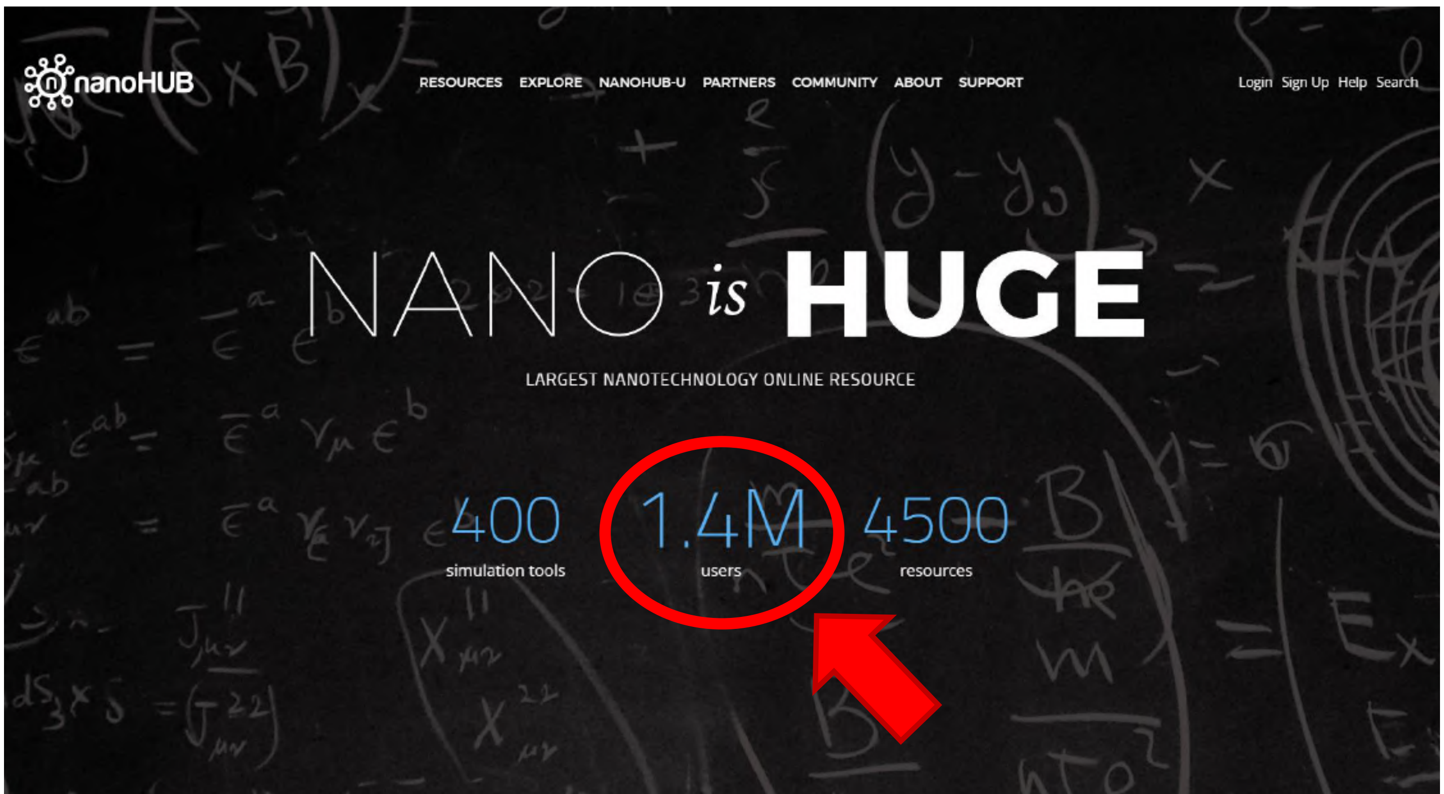
The NanoHub project

www.nanohub.org

NCN

PURDUE UNIVERSITY

Ale Strachan



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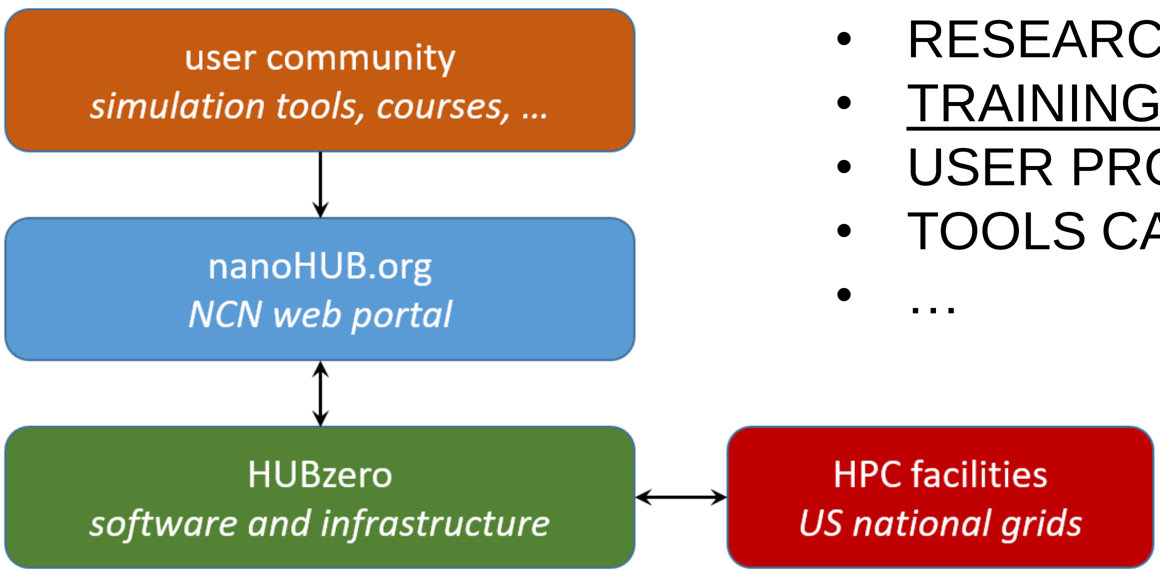
How does it work?

Online platform for community-contributed simulation tools for science and engineering, with particular focus on nano-technological problems and applications.



- RESEARCH TOOLS
- TRAINING TOOLS & MATERIAL
- USER PROFILING
- TOOLS CAN BE CITED (DOI)
- …

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Online training opportunity

Search: Pietro Asinari

Results (page 1 of 1)

Pietro Asinari

Members

bio

+ *Online Presentations (1)*
+ *Tools (1)*

https://nanohub.org/members/129830

Multiscale Modelling of Nanoparticle Suspensions

Online Presentations 12 Jun 2017 Contributor(s): Pietro Asinari

Self-assembly of nanoparticles (NPs) into mesoscopic ordered structures plays a crucial role in a large variety of applications including pharmaceutical, food, drug delivery, immunology and technological. On the one hand, trying to prevent and avoid the self-organization of nanoparticles has traditionally been the main issue for stabilizing nano-...

https://nanohub.org/resources/26710

THERMAL CNT

Tools 22 Aug 2017 Contributor(s): Luca Bergamasco, Matteo Fasano, Eliodoro Chiavazzo, Pietro Asinari, Annalisa Cardellini, Matteo Morciano

This software computes thermal conductivities of single-wall carbon nano-tubes (SW-CNT) via NEMD (non-equilibrium molecular dynamics) method. Two versions of the same program are available: a tool version for fast set-up and simulations and a step-by-step tutorial for students. The procedure used to compute the conductivity is outlined in the...

https://nanohub.org/resources/tcnt

By Pietro Asinari

Department of Energy, Politecnico di Torino, Torino, Italy

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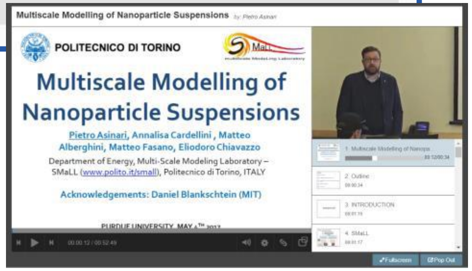

28 users

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Online tool (app) profiling

www.nanohub.org/tools/tcnt

THERMAL CNT

By Luca Bergamasco[1], Matteo Fasano[1], Eliodoro Chiavazzo[1], Pietro Asinari[1], Annalisa Cardellini[1], Matteo Morciano[1]

1. Politecnico di Torino

Compute thermal conductivity of single-walled carbon nano-tubes via NEMD method

Launch Tool

Version 1.0 - published on 22 Aug 2017

doi:10.4231/D3J678Z8J cite this

This tool is closed source.

View All Supporting Documents

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Cite this work

Researchers should cite this work as follows:

Luca Bergamasco; Matteo Fasano; Eliodoro Chiavazzo; Pietro Asinari; Annalisa Cardellini; Matteo Morciano (2017), "THERMAL CNT," https://nanohub.org/resources/tcnt. (DOI: 10.4231/D3J678Z8J).

BibTex EndNote

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Brief wrap-up

- NanoHub is interesting also as a prototype marketplace
- Modelling apps allow more user-friendly use of materials modelling
- Putting modelling apps on the same platform force them to respect the same standards, prone to interoperability
- Interactive notebook software (e.g. Jupyter) helps to deliver materials modelling also to non-experts (e.g. economical decision makers)
- Modelling apps can automatically produce success stories, if users allow disclosure

- Online material can be used for training, maybe also for economic training
- Ideal for Massive Open Online Courses (MOOC)

Test cases (more on neutrality)

Selected translation test case 1:
long-term client/translator collaboration example

Manuel Laspalas, ITAINNOVA (ES)

Selected case from survey: the problem

- **Translator:** technological (consultancy) centre
- **Client:** large company of the automotive sector

- **Problem:** The problem was related to the morphology development (mainly fiber orientation) during the manufacturing (injection process) of a component made of short fiber reinforced plastic, and its effect on the functional performance on the product (elasticity and strength).

- **Has the client CAE experience/department:** yes
- **Why do the client need a translator?** They mainly use their CAE resources for supporting the design and development process of components. They use translators to extend functionalities of the simulation workflows to new problems or to consider new aspects.

Selected case from survey: comment on neutrality

- **Did you know the company in advance?** Yes, long relation with the company, that for the problem in question started with experimental analysis projects.
- **Did you propose to the client only one or several places/groups where modelling/simulation can be executed?** One, us, because in our case we are executors
- **Did you propose to the client only one or a number of potential software tools or solutions?** We proposed and investigated several different solutions and software at the beginning of the long-term collaboration with the company. Now that we know the company very well, we tend to use well assessed methods and tools

COMMENTS ON NEUTRALITY

If a translator is also executor, "external" neutrality is very difficult

"Internal" neutrality comes during first approach of the client

Selected translation test case 2: good translator's neutrality example

Adham Hashibon, Fraunhofer (GE)

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Selected case from survey: the problem

- **Translator:** non-for Profit Research organisation
- **Client:** Material Producer, manufacture equipment supplier
- **Problem:** Tuning processing parameters under real manufacturing conditions
- **Has the client CAE experience/department:** no
- **Why do the client need a translator?** Since they do not have experience with modelling

Selected case from survey: comment on neutrality

- **Did you know the company in advance?** No, first contact through initial telephone contact

- **Did you propose to the client only one or several places/groups where modelling/simulation can be executed?** Multiple, that can collaborate on the solution (the company choses based on price); we were involved in modeling tasks upon request of the client

- **Did you propose to the client only one or a number of potential software tools or solutions?** Software tools are explicitly not part of the translation process. The modeler decides which tool to use

COMMENTS ON NEUTRALITY

In this case several choices for the SW and execution are given

Here the modeler should provide further options for tools

Update on model gaps

MODEL GAPS: overview

OBJECTIVE: Assessing the capability of existing models and finding the model gaps to be filled according to industrial needs

More in detail, the goals are to:

- **Identify model gaps** and
- **Establish Roadmaps** to cure them and to
- **Assess their errors/accuracy** (verification),
- **Validate the models** (validation)

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MODEL GAPS: recent activities

- Web-based survey
  - collected input on the status of key topics needing action in Europe
- eSSENCE-EMMC Multiscale modelling meeting in Uppsala 12-14 June 2017 on "Multiscale modelling of materials and molecules“
  - Data-driven or physics-driven models?
  - Modelling as a characterization tool.
  - Molecular dynamics simulations and sampling techniques.
  - From electronic calculations to atomistic models and coarse-grained simulations
  - Along the multiscale ladder + accuracy and validation.
- EMMC Focused workshop in Uppsala 15-16 June 2017 on "Model gaps and widening models for industrial needs“
  - Model gaps – identification and remedies
  - Accuracy and accuracy assessment: The human error, the systematic error and the statistical error
  - The roles of software developers and translators in these efforts
  - Economic impact of modelling

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MODEL GAPS: the 2016 web-survey

- 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).

	Importance	Urgency	Importance x Urgency
	Low number means more important		
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

MODEL GAPS: outcome of the 2016 web-survey

- **Request: Better discrete models**
  - Almost all of the participants in the survey listed available discrete models are insufficient or lacking and hence model development is needed.
  - 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.

- **Request: Better Coupling / Linking models and workflows**
  - Model-wise C/L needs among the discrete models are 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.

Recommendation of areas for model improvement (i.e. where gaps are identified)
The following model gaps and adhering areas were among those repeatedly brought forward at the meeting:

1. The *soft matter* sector (see next slide) is an economically strong area in Europe. Here modelling requires very long simulation times; consequently good *atomistic* models are crucial, but they are to a large part lacking.

2. Also the industrially important *semiconductor electronics* (see next slide) sector needs modelling results. Here both the continued development of accurate *electronic* models is and atomistic models for process simulations of some hundred thousand atoms are important. Reliable models are needed.

3. Other models are important to the *(Sector S1) automotive/aviation metallurgy*, e.g. to simulate crystal plasticity where material microstructures must be captured correctly, and high fidelity is required for models of failure initiation and crack propagation involving e.g. twins and grain boundary precipitates.

4. Close interaction between model development and experiment is needed and this development is looking quite promising.

MODEL GAPS: recommendations from Uppsala (I)

Summary of recommendations from the two Uppsala meetings

1. *(S2) Heterogeneous catalysis*, *(S3) microelectronics*, materials modelling for *(S4) drug discovery & nanosafety*, and *(S5) interfaces including functional materials and composites (example of collaboration with EMCC)* and are four topics where the roles of discrete models are vital. Here models and workflows – not least involving coupling and linking of materials models - are gradually becoming more reliable, but the predictive power is still often limited.

Recommendation 1a: Follow-up with exploration of the details of the requirements raised in these areas, and with further endorsement.

Recommendation 1b: Brainstorm with the EMMC communities to find a form and forum to support the time-consuming development of models towards predictability.

2. Several success stories of high added value and probable return of investments (economic impact) thanks to modelling were reported.

Recommendation 2: As a joint effort between WP1, WP4 and WP5 follow up for more elaborate reports and in a form which can be made public.

3. Materials *properties* with known and *adequate* accuracy are key to the acceptance of computational materials research by the industry.

Recommendation 3a: Make closer contacts with the Materials Characterization Council.

Recommendation 3b: Provide success stories to industrial partners.

MODEL GAPS: recommendations from Uppsala (II)

Summary of recommendations (cont.)

4. The role of materials informatics and automated and/or data-driven model development is clearly escalating rapidly. Recommendation 4: Elaborate methodologies to explore further the relation between data driven models and physics-based models and their relative potential impact on industrial modelling, challenges and benefits.

5. The lack of adequately accurate models (=> skepticism) and efficient models (=> slow) models and workflows is a (if not the) main barrier to a breakthrough of materials modelling in industry. However, several other types of barrier are also relevant here, e.g. lack of training, lack of controlled experimental data for validation, lack of validated workflows, etc.

Recommendation 5a: Discuss and clarify expectations of industrial partners with respect to accuracy and efficiency.

Recommendation 5b: Provide a list of realistic expectations concerning accuracy and efficiency as a benchmark for model developers, code developers and software owners.

Recommendation 5c: For efficient information passing, keep up the active information interchange between the various EMMC WPs and communities.

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METHODOLOGY: Template for model gaps?

A Study Organized by The Minerals, Metals & Materials Society on behalf of the National Institute of Standards and Technology (NIST) Material Measurement Laboratory

Modeling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales

- Different nomenclature (USA) but interesting methodology?
- How to make such assessment more objective?

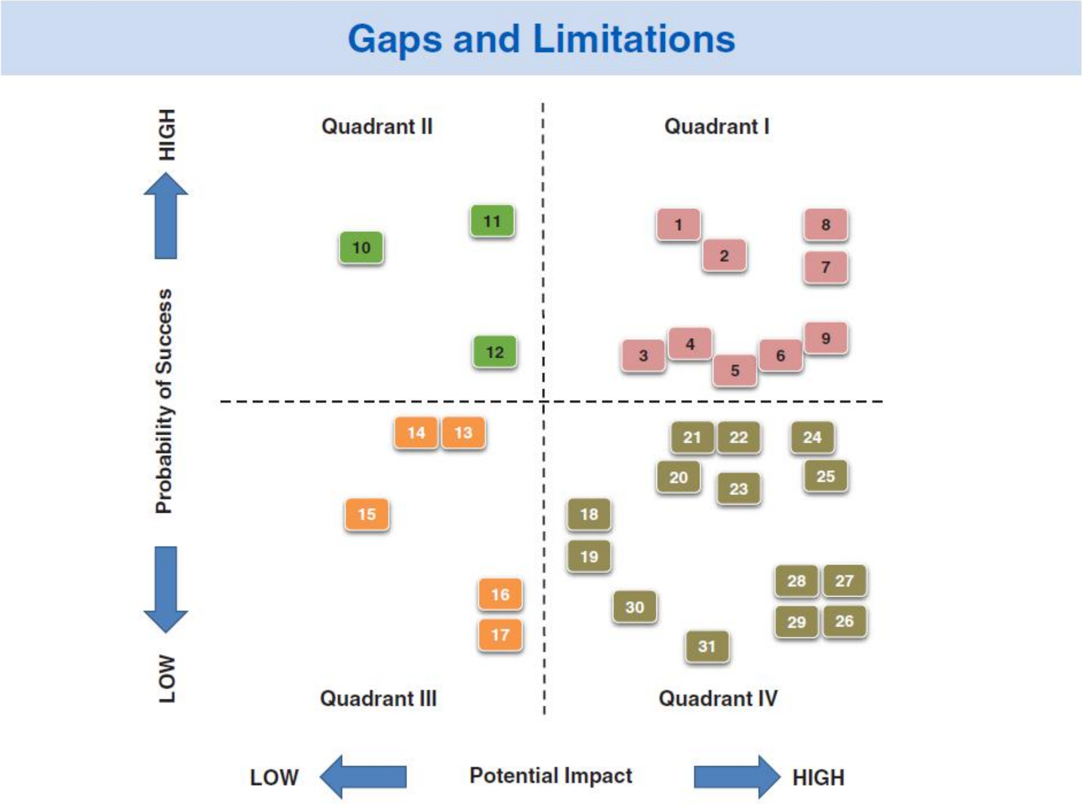

Figure: Gaps and Limitations for Modeling Across Scales

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