Artificial intelligence based tools to support translators in material modelling: The ongoing training test case at Politecnico di Torino and Politecnico di Milano

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Brief overview

• Our research lab;

• Translator profile and the envisioned training scheme for translator with possible criticalities;

• Translator role in industry digitalization;

• The ASP (Alta Scuola Politecnica) project: A joint effort of Politecnico di Torino and Politecnico di Milano to support translators in the near future.
Heat & mass transfer:
1) Solar Energy
2) Energy Storage
3) Clean Water

Multiscale modeling
- Atomistic (MD)
- Coarse Grained (CG)
- Mesoscopic (LBM)
- Continuum (CFD)

Rapid prototyping
- Solar thermal energy
- Sustainable water treatments
- Heat storage
- Enhanced heat transfer
Our research group

- Pietro Asinari, PhD Full Professor
- Eliodoro Chiavazzo, PhD Associate Professor
- Matteo Fasano, PhD Senior Researcher
- Luca Bergamasco, PhD Post-doc
- Annalisa Cardellini, PhD Post-doc
- Matteo Alberghini, PhD candidate
- Paolo De Angelis, PhD candidate
- Matteo Morciano, PhD, Post-doc
- Rajat Srivastava, PhD, Post-doc
- Post-doc to be hired soon
Our teaching duties

- Six undergraduate courses delivered by our group members (5 at master level + 1 at bachelor level). Courses are on 1) Advanced Engineering Thermodynamics (3 parallel courses in Mechanical Engineering); 2) Energy storage (1 course in Energy engineering); 3) Energy applications of materials (1 course in Energy engineering); 4) Applied Thermodynamics and Heat Transfer (1 course in Mechanical Engineering);

- This amounts to **over 500 students** every year enrolled in our courses;
Translator profile as identified by the EMMC is complete and meets exactly the expectations on their role in industry?

References:

- EMMC Translators Guide
- EMMC Survey (presentation) on Translation & Training for marketplaces:
- EMMC YouTube channel (economic training videos)
  [https://www.youtube.com/c/europeanmaterialsmodellingcouncil/](https://www.youtube.com/c/europeanmaterialsmodellingcouncil/)
- iMat project @Alta Scuola Politecnica
Translators have the capacity of “translating” industrial needs into well posed modelling task that are understandable by specialists in academia, thus overcoming the “language” barrier;

However, we should never forget that academia and industry are separated not only by the language, but also (and sometimes most importantly) by objectives and mission;

Academicians are typically interested in scientific advancements and publications which are the main items evaluated for career advance. Completely different criteria are usually requested in the industry;

If translators have to really talk to those different “worlds”, their training should also provide a deep knowledge on mechanisms behind career advancements in different environments. Effective solutions/rewards to facilitate and motivate the collaboration are necessary;
The Training scheme for Translators identified by the EMMC is sufficiently complete?

- The Training for Translators is intrinsically **multidisciplinary** and should include: 1) Wide technical background; 2) estimation of economic impact on modelling; 3) estimation of investment vs benefit; 4) soft skills;

- However, the judgment of Translators should never be biased by always considering modelling as the only possible solution (i.e. let’s avoid the **Maslow's hammer**);

- Hence, as far as the wide technical background of the translator is concerned, this should not only focus on the several modelling tools, but also include some additional expertise on alternative tools for decision making (e.g. **data analysis**, high-throughput experiments, design of experiments, surveys,…);

- Decisions not necessarily (i.e. not always) require a modelling-based support, and a more comprehensive profile is an important guarantee of fairness, neutrality and credibility of Translators;
Critical aspects in training of translators?

- The training for translators is intrinsically multidisciplinary and could/should rely upon specially designed courses, where lecturers from multiple disciplines (both from industry and academia) are harmonically orchestrated by scientists/experts with a broad multidisciplinary background;

- However, as far as the academic world is concerned, truly multidisciplinary curricula are still rather exceptional among scientists;

- To some extent, the above difficulty has still to do with the career progression in the academia (evaluation and comparison of multidisciplinary profiles is much more complicated and less established);

- Owing to its intrinsic (multidisciplinary) nature, a possible critical aspect to be considered for translator training could be the need for refresher courses;

- Artificial intelligence tools and automatic reviewing of large body of literature data (see iMat project below) might help in making all this more cost-effective.
Translators can have a central role in the digitalization

• Translators will most probably play a critical role in the transition towards the European industry 4.0;

• A more flexible manufacturing system will be characterized by a larger number of “translation problems”. This can specifically (and negatively) impact on SMEs (due to a lack in expertise diversity and a limited budget for research activities);

• Automated tools for a systematic analysis of literature data (see iMat project below) can play an important role in the future especially for SMEs. It is possible to envision some future scenarios, where very few internal translators (possibly only one) supported by powerful AI-based tools can sustain a sufficient level of innovation in SMEs;
Additional training concepts that may be useful to provide to the Translators towards industry 4.0?

• Translators should be familiar with modern tools for data mining and machine learning in order to develop abilities in handling large heterogeneous (i.e. of different origin e.g. from simulation and experiments) data. This enables to possibly have decisions based on data-driven models when physics-based models are either too demanding or not sufficiently accurate;
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«Alta Scuola Politecnica» – ASP in a nutshell

- **A joint venture** between the largest and oldest technical Universities in Italy. Established in 2004, two-year study cycle, 15th cycle starting in 2019;

- **150 talented students** per year, selected among the best applicants to the Master programs in Architecture, Design and Engineering;

- **On-top program**, additional to master studies;

- **Articulated teaching**: 4 one-week residential programs, long and short seminars, hands-on multidisciplinary project work.

[http://www.asp-poli.it/](http://www.asp-poli.it/)
ASP: An intrinsic multidisciplinary initiative

ASP Students School in the 15 Cycles (2004-2018)
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ASP: Excellence track

Standard education path

- PhD
- MSc
- BSc

Excellent students

Multidisciplinary teams

Projects proposed by academic tutors

Academic tutors
iMat project (ASP): Taking advantage of AI tools

Review of material properties via automatic literature screening and data extraction

**Translator 2.0**: exploit artificial intelligence for industrial innovation (Test case: literature analysis of materials for Thermal Energy Storage, such as zeolites)

Please visit us at: https://imat-asp-project.com/
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The iMat Project Team

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Project at a glance: The vision

1. Research papers from Industrial and Academic research are collected.

2. Data about chemical compositions and related properties are extracted.

3. Data are used to train Machine Learning Algorithms.

4. ML is used to identify patterns able to correlate and foresee properties from chemical compositions.

https://imat-asp-project.com/
Artificial Intelligence covers two main roles in the process:

**Data Extraction**

It is able to go through thousands of papers and **recognise** valuable information to collect and gather in a database specific for the particular topic.

**Innovation Forecast**

It will then provide **recommendations** on most promising chemical compositions to lead the research and company’s investments with increased awareness.
“Which zeolite-based microporous sorbent* is the most suitable for a Thermal Energy Storage application using water as sorbate?”

*By zeolites we refer to a wide family of microporous materials. Some of those materials are characterized by both high surface area and (water) adsorption heat, and can be used as solid adsorbents for Thermal Energy Storage (TES) applications. Selection of optimal sorbents allowing storage of renewable heat is essential to overcome one of the major limitations of renewable energies, namely intermittence.
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The process. Still ongoing effort…
We intend to reach 5000-10000 articles joining different sources (mostly for data extraction not training)
Currently evaluating extraction from patents

Example:

- heat of adsorption: 79.5 kJ/mol
- micropore size: 0.55 nm
- surface area: 310.83 m²/g
Paradigm shift

**Decision**

- Translator 2.0 will have to carefully select the training data and for that can be helped by specialists;
- Translator 2.0 will mostly supervise the training phase of AI tools;
- Once the AI tools has been trained they can be possibly shared among SMEs
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