An Open-Innovation Platform for knowledge-based management of materials modelling workflows for industrial data

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1. Introduction

Understanding the properties of complex materials through materials modelling has been the drive for intense research in the field of numerical simulations for almost 100 years [1]. The advances made in computer hardware and simulation software now allow capturing the behaviour of materials down to any desired/required level of interactions (continuum, mesoscopic, atomistic or electronic) and at scales extending from nano- to macroscopic. Modern computational materials science relies heavily on automated complex numerical procedures, involving multi-step processes and on the integration of different simulation software. While workflow managers exist to automate, execute, and track materials modelling workflows, a steep learning curve still exists for utilising materials modelling effectively. Moreover, multi-model/multi-scale simulations coupling or linking different models and operating at different length and time scales require a level of expertise that is rarely mastered by a single individual. Finally, reproducibility of numerical simulations and validation of modelling strategies are often poorly addressed in the published literature, e.g. by lack of a standard format for sharing technical details. Therefore, the need arises to better manage, document and retrieve workflows, exposing the physical predictions to end-users without prior knowledge of theoretical models or specific software.

2. The OpenModel platform

The Open-Innovation Platform developed in the OpenModel project [2] addresses the challenges of managing materials modelling workflows by using semantic technologies for storing, documenting, retrieving, and executing them. An ontology-based simulation platform has been developed, which includes a workflow ontology, a big-data curation database, integration of third-party software, and a workflow runner/executor. The OpenModel platform delivers accurate, validated, and traceable simulation workflows and uses ontologies to formalise the knowledge required to use materials modelling. On top of that, a semantic description of input and output datasets delivers Findable, Accessible, Interoperable, and Reusable (FAIR) data which are fundamental for the

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digitalisation of industry. Validation and verification of materials workflows are performed with dedicated software, and the results attached to the workflows as metadata. In this way the platform ensures the consistency of numerical predictions and the robustness of materials models.

3. Workflow Builder

The OpenModel software stack includes a semantic-based workflow builder that describes workflows as tasks exchanging datasets. This information is stored in a knowledge base and retrieved using high-level queries. It enables end-users to initiate computations without detailed knowledge of computational implementations. In case of conflicting requirements, an algorithm prioritises and supports selection among potential workflows. The exchange of data between tasks is provided by pipelines based on semantic mapping schemas plus parsing and serialisation plugins. By storing workflows and datasets semantically in a knowledge base, new simulation workflows can be obtained as the builder can infer connections between heterogeneous tasks, providing new insights into complex problems. The builder utilises the Elementary Multiperspective Material Ontology (EMMO) [3] as a conceptual framework for describing workflows at various levels of detail.

4. Workflow Management

The materials modelling workflows are executed using the AiiDA [4] Python infrastructure. The validation and verification services assess the logical consistency and integrity of workflows, ensuring accuracy in physical predictions by comparing simulation outputs to reference data. This approach enhances the creation of reliable and reproducible materials modelling workflows, crucial for informed decision-making in industrial contexts and for FAIR datasets creation from simulation outputs, which can be used to interpret experimental data or for machine learning applications. By embracing semantic technologies and FAIR principles, OpenModel facilitates seamless integration and sharing of materials modelling data, contributing to the advancement of digital economy principles and Industry 5.0 initiatives.

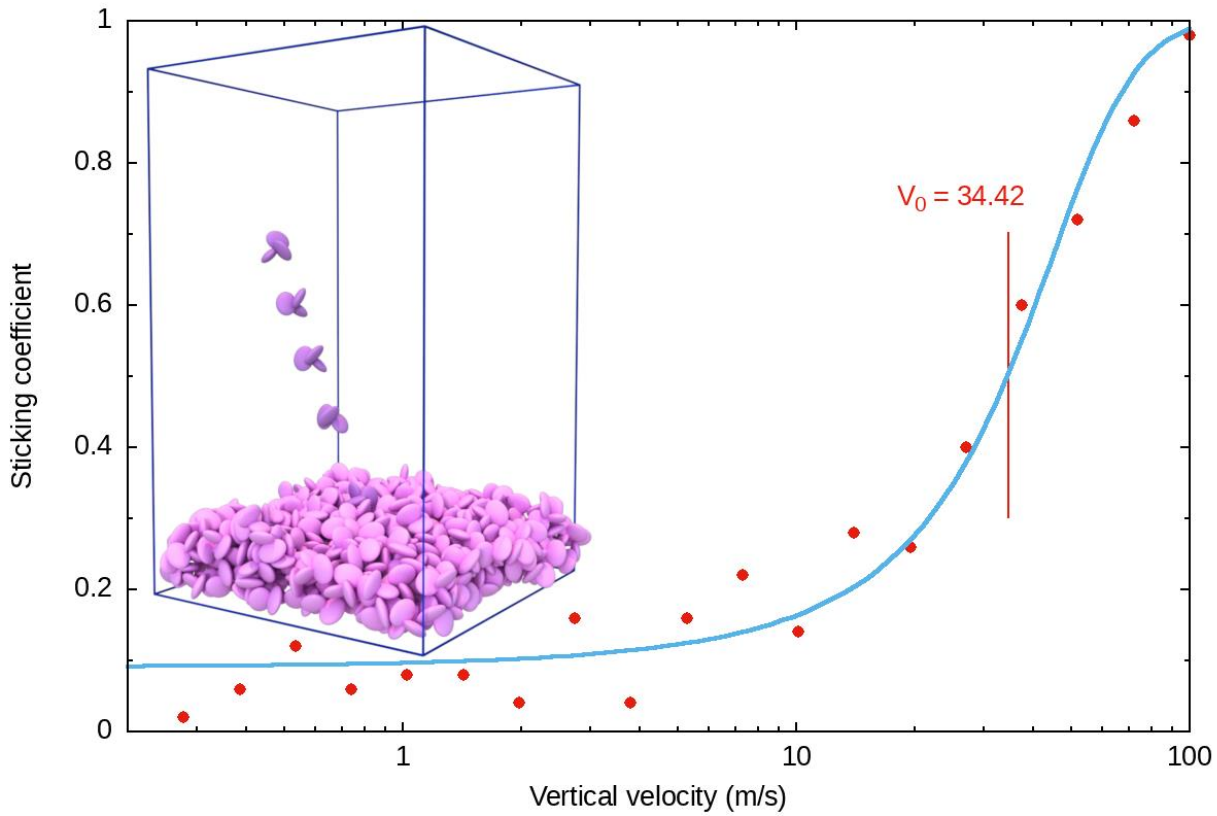

Figure 1: Extracting physical observables from molecular simulations involves setting up materials models, executing specialised software, and post-processing the resulting data. Managing these complex workflows and connecting them to metadata describing their physical accuracy and numerical consistency are among the objectives of the OpenModel project.

5. Conclusions

The OpenModel project has developed an Open-Innovation Platform which enables a knowledge-based approach to materials modelling workflows for industrial data. By leveraging semantic technologies, the project enables efficient management, validation, and sharing of simulation workflows, ultimately bridging the gap between industrial challenges and actionable results. Through the creation of FAIR datasets and adherence to best practices, OpenModel fosters a collaborative environment promoting innovation and informed decision-making in materials science and the manufacturing industry.

6. References

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[2] OpenModel project: https://open-model.eu/

[3] Elementary Multiperspective Material Ontology: https://github.com/emmo-repo/EMMO

[4] M. Uhrin *et al.*, *Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows,* Computational Materials Science **187**, 110086 (2021); DOI: 10.1016/j.commatsci.2020.110086

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