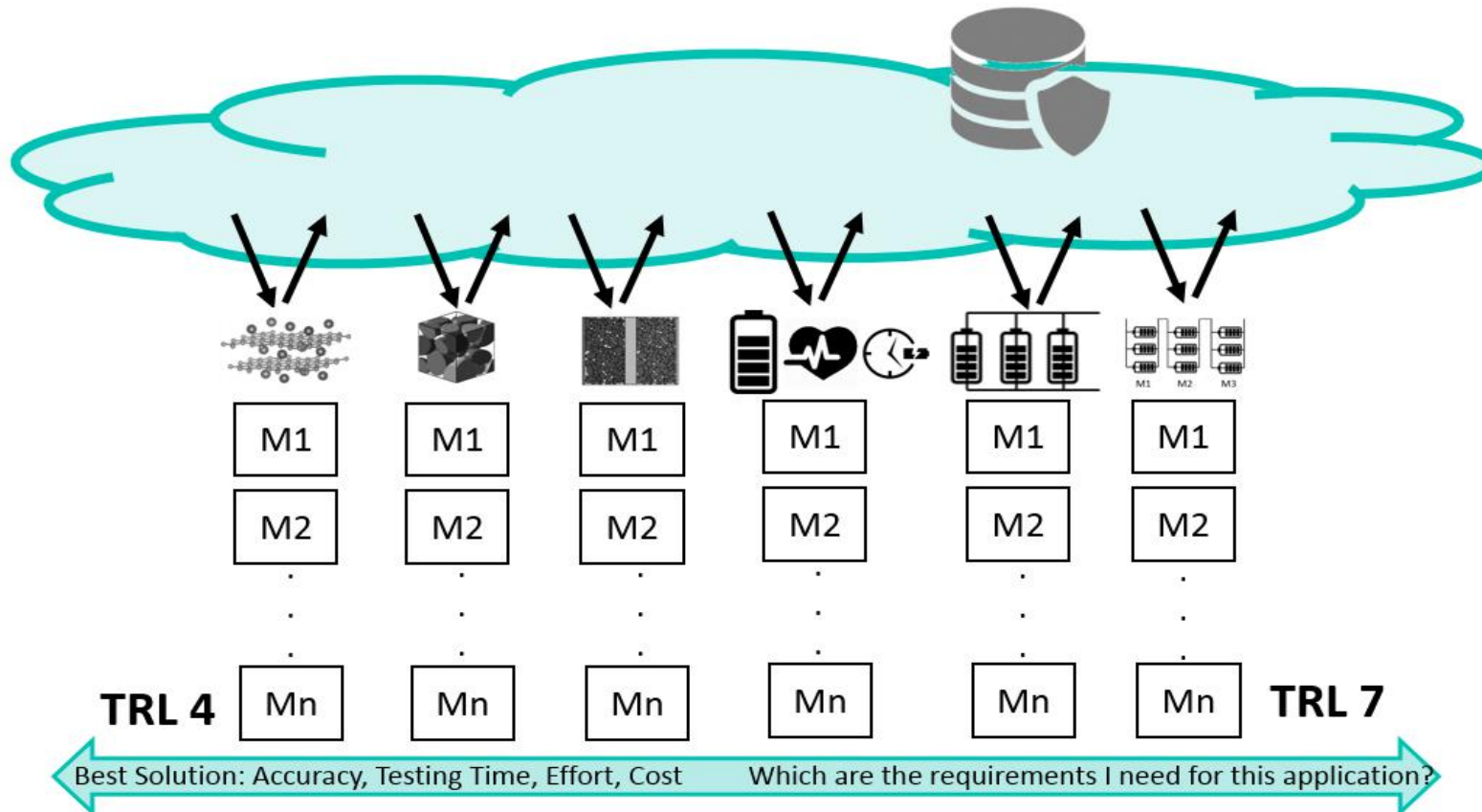


IMMENSE:

Integrated and Interoperable Multiscale Modelling Solution for Electrochemical Energy Storage System.

The project will develop a **novel, standardized, interoperable and industry-ready software solution for the modelling and prediction of present and next-generation materials and batteries for a wide range of applications.**



State-of-the-Art

- **Interoperability and user-friendliness**

State-of-the-art:

The UNICORE middleware provides a user-friendly workflow editor in the graphical Rich Client.

The workflow engine, the data access and job execution are all implemented as an interoperable RESTful web services.

The FireWorks workflow system:

- Implemented with lightweight components (simple Python API Commands)
- Highly interoperable document database MongoDB.

Challenges:

- Lack of a domain specific language for multiscale and multiphysics modelling and related tools
- Limited interoperability at the semantic level and user-friendliness
- Limited acceptance and adoption in the materials research community.

Progress beyond state-of-the-art:

- The **IMMENSE** project will bridge this gap with developing domain ontology for full-scale battery modelling relying on **European Materials Modelling Ontology (EMMO)** currently developed by the EMMC-CSA project.

Semantic Interoperability, HOW?

Concurrent strategies will be followed, by:

- Extending the integrated software with wrapper tools to ensure basic compatibility at the taxonomic.
- Using hierarchical dictionaries to describe and harmonise the interfaces of integrated code.
- Exploiting and extending the **European Materials Modelling Ontology (EMMO)**, currently developed by the EMMC-CSA project, which will provide a higher level of semantic interoperability in a longer-term perspective.

The overarching **EMMO** will be extended with a domain-specific ontology covering the modelling on the electrode, electrolyte, cell, module and battery-pack levels.

<https://emmc.info/about-emmc-csa/>

