The 8th European Congress on Computational Methods in Applied Sciences and Engineering
ECCOMAS Congress 2022
5–9 June 2022, Oslo, Norway

RELIABLE MATERIALS MODELLING TRANSLATION FOR INTERFACIAL AND TRANSPORT PHENOMENA

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Keywords: *Simulation Workflows, Provenance Metadata, Reproducibility, Translation*

Digital infrastructures in materials modelling can contribute to improving reproducibility and reliability in molecular simulation. Metadata standards for modelling and simulation *data provenance* can facilitate *reproducibility and trust* in data, while automated and assisted annotation of simulation outcomes, integrated into workflow management systems, can reduce the amount of *dark data*. Parameterizing bespoke molecular models by multi-criteria optimization can improve model accuracy with respect to interfacial and transport properties, at the expense of other properties. Such efforts support the knowledge transfer strategy known as *translation* in materials modelling, which was formulated by EMMC ASBL and has found a substantial uptake. This contribution reviews recent progress along these lines, with a focus on perspectives for platform interoperability and cross-platform collaboration targeting thermodynamic properties and processes involving fluids at interfaces. The relevant infrastructures include *digital marketplaces* such as VIMMP and DOME 4.0 (and MarketPlace, Market4.0, etc.), *open innovation platforms* such as VIPCOAT (and OpenModel, etc.), and model repositories such as MolMod DB. It will be explored what the main use cases from these platforms, such as active protective coatings, have in common. This also concerns large-scale *research data infrastructures*, including UKRI EPSRC funded work on a Physical Sciences Data Infrastructure and disciplinary consortia from the German NFDI programme, many of which aim at contributing and adhering to agreed good practices and recommendations within the framework of EOSC.

H2020 GA no. 721027 (FORCE), 760907 (VIMMP), 952903 (VIPCOAT), 953163 (DOME 4.0).