TITLE: Molecular Informed Large-Scale Simulations

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ABSTRACT:

In this talk I will present the Siemens portfolio of multiscale modelling tools and our renewed technology development roadmap. I will discuss the ambitions in “multi-scale design for new production technologies”.
I will then focus on “Molecular informed Large-Scale simulation” which is a new direction we are launching. Chemical & process companies cater to a wide range of industries such as aerospace, automotive and consumer products. Materials produced by the chemical industry needs to be tightly linked to the product requirements of their customers in parts or formulations productions. This calls for a better integration of different field of science from chemistry to chemical engineering and processing and design, geometry, or material science. I will describe how we intend to develop a molecular simulation approach to start addressing this issue.
Finally, by combining our competences in AI and materials science and leveraging efficient approaches developed in small molecule[1,2,3] data analytics, I will present a new approach based on hierarchical graph embedding that allows the "digital synthesis" of chemical molecules (including polymers) that satisfy requirements of thermodynamic and physicochemical properties. This will be demonstrated as an efficient approach to feed a large-scale simulation with molecular details.
Using molecular level simulations and publicly available chemical database, I will demonstrate the validity of our approach on common chemical properties. We demonstrate our process on publicly available databases.

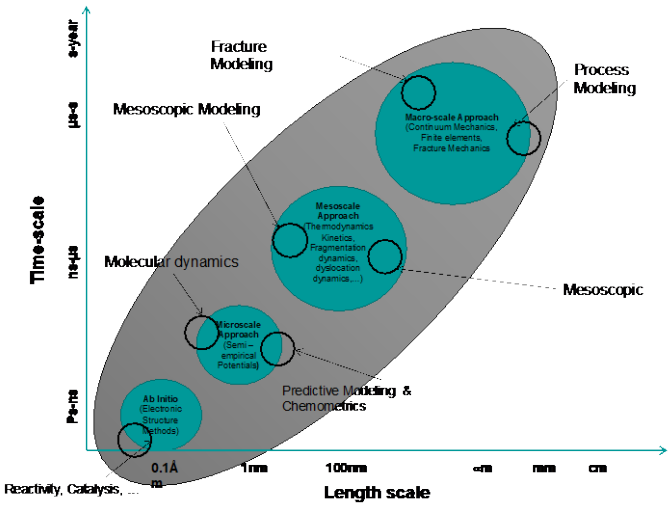

Figure 1: Multiscale modeling paradigm.

References

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