

Beyond the Particle Ladder: Integrative Multiscale Modelling from Electrons to Digital Twins

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Multiscale modelling ladder in chemistry, materials science, and biosciences is often presented as a particle-based hierarchy, where electrons and nuclei are converted into atoms, atoms into molecules, molecules into coarse-grained beads, and beads into larger effective units. We will discuss a broader and more powerful view [1]. Once particles become too coarse for meaningful building blocks of matter, multiscale modelling must continue through fields, free-energy functionals, equations of state, hydrodynamics, pore networks, population balances, process models, digital twins, and data-driven inference [2,3]. We will here picture an integrative roadmap. connecting bottom-up molecular modelling with top-down experimental, thermodynamic, and engineering constraints, highlighting how methods from chemical engineering, applied mathematics, computer science, AI, inverse problem solving, and experimental characterization can be combined into a coherent modelling strategy [4]. The message is that modern multiscale modelling is not simply coarse-graining across length and time, but the systematic transfer of information across representations, observables and decisions.

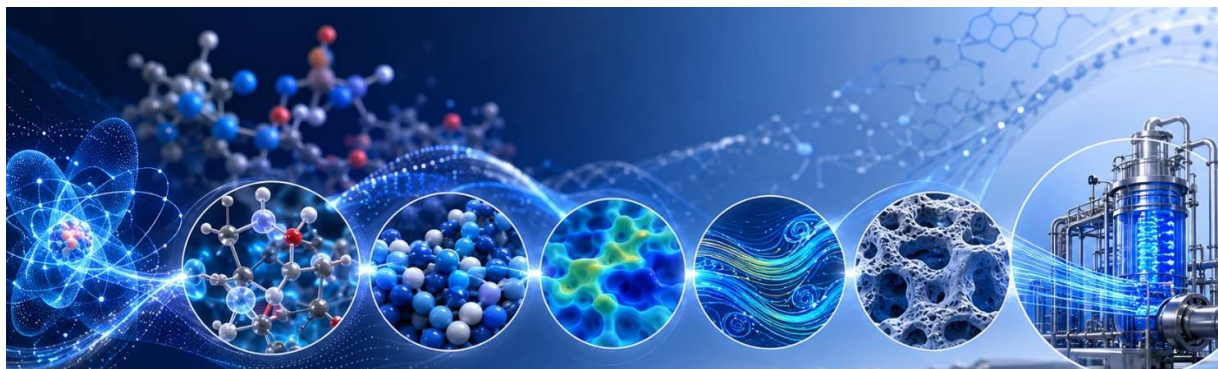


Figure 1 - A generic multiscale scheme from electrons to industrial processes where information is passed from one scale to the next

REFERENCES

- [1] E. W. and Engquist, B. *The Heterogeneous Multiscale Methods*. Communications in Mathematical Sciences **1**, 87–132 (2003).
- [2] Mane, S., Dhote, R. R., Sinha, A. and Thirumalaiswamy, R. *Digital twin in the chemical industry: A review*. Digital Twins and Applications **1**, 118–130 (2024). DOI: **10.1049/dgt2.12019**.
- [3] Thelen, A. et al. *A Comprehensive Review of Digital Twin — Part I: Modeling and Twinning Enabling Technologies*. arXiv:2208.14197 (2022).
- [4] Alexander Lyubartsev, Aatto Laaksonen, Hierarchical Multiscale Modeling Through Inverse Problem Solving, in Comprehensive Computational Chemistry, Volume 3, 2024, Pages 622-635 <https://doi.org/10.1016/B978-0-12-821978-2.00121-5>