

Multi-scale multi-physics approaches for accurate simulations of complex chemical systems.

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Predicting the behavior of real macroscopic system from its basic chemical constituents has always been one of the ultimate goals of computational chemistry. Multi-scale multi-physics based approaches present a natural evolution of conventional computational chemistry applications. These methods recognize natural decomposition of the chemical system into distinct regions (multi-scale) and the advantages, both computational and conceptual, of the integrated approach that uses different theoretical models (multi-physics). The latter descriptions could be associated with different parts of the overall chemical system and/or can coexist in the layered fashion. Several examples of multi-scale multi-physics applications will be presented ranging from finite temperature excited states to free energy calculations in chemical and biological systems.

References

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^{*}Pacific Northwest National Laboratory, EMSL, Richland, WA, 99352. Research supported by DOE ASCR Multiscale Mathematics program.

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