
Perspective

An Historical Perspective

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The unrelenting advance of computing power that is available to physical scientists has produced remarkable changes. In theoretical chemistry alone, it has magnified opportunities for quantitative prediction, and for rational organization and analysis of huge databases. These general trends have been obvious. Perhaps slightly less obvious is the desirability and need to establish strong communication and collaboration links between the communities of theoretical and computational chemists on the one hand, and the broad mathematics community (including pure, applied, and computer science scholars) on the other hand. Ideally, such linkage would exhibit a kind of intellectual symmetry, with novel concepts and suggestions for untapped research ideas flowing both ways.

With that idealistic vision as background, the National Research Council (NRC) initiated a study just over a decade ago to survey the prospects for, and barriers to, such interdisciplinary interaction. The committee chosen for this task was selected from the chemical community alone, although one could have imagined including representatives from mathematics as well. Its deliberative efforts culminated in a publicly available report [Mathematical Challenges from Theoretical/Computational Chemistry, National Academy Press: Washington, DC, 1995]. While this report did not claim to have made an exhaustive examination of its subject,

it nevertheless found compelling grounds for expanding opportunities in interdisciplinary research at the chemistry–mathematics interface, and proposed concrete actions to reduce or eliminate barriers to such opportunities.

The 1995 NRC report concluded with an Afterword urging that after 5 years had passed its subject should be revisited. The hope was to gauge the extent to which its observations and recommendations had made an impact, and to judge whether any key features had been missed by the report's authors. Hindsight makes it clear that the revisitation suggestion was overly optimistic with respect to timing and to breadth. But now that twice the suggested 5 years has elapsed, it is satisfying to see that the present focused issue of the *International Journal of Quantum Chemistry* has highlighted one productive area of interdisciplinary cross-fertilization, specifically symbolic calculation. Perhaps there is now reason to expect that other mutually beneficial contact areas involving theoretical/computational chemistry and mathematics will receive similar focused attention. Both disciplines stand to benefit handsomely.

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