Brief history of computational chemistry: Three distinct eras and the relative importance of theoretical insights and computing power in advancing the field

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Abstract

The past influence the present and future; for example, in computational chemistry, simplifying assumptions and approximations critical to problem-solving in the pre-computing era remains relevant today in allowing simulation of larger systems with reasonable amount of computational time. By highlighting significant milestones in efforts - from both theoretical and simulation perspectives - aimed at understanding the nature of chemical bond formation, this abstract-only preprint describes a short essay that traces the development and evolution of electronic structure calculation methods over the years, as well as demystify many of the field's technical terms (jargons) and eponymous method names that has presented a significant entry barrier to newcomers. Schrodinger equation occupies central place in computational chemistry, where the focus was, and will continue to be, the development of methods for its solution. Placing the various methods along a time-line and observing the temporal relationships between them, reveals the clustering of methods into three distinct eras, each defined by their relative reliance on theory, approximations, experimental data and computational power for problem solution. Specifically, building of theoretical models for explaining spectroscopic emission spectra laid the initial foundation of the field when theory lagged behind experimental observations. Promulgation of the Schrodinger equation – which describes total system energy and properties via a quantum mechanical framework - shifted the research focus of the field towards its solution. Nevertheless, difficulty in solving the equation during the pre-computing era spawned an entire sub-field seeking to develop increasingly refined methods for obtaining approximate solutions. Specifically, semi-empirical methods rely on experimental data to supply parameter values inaccessible via direct calculations from first principles, while approximate methods use simplifications, for example, to obviate the need for calculating cross-interacting terms. Availability of large amount of inexpensive computational power in recent years, however, brought forth *ab initio* (first principles) simulation methods capable of calculating electronic structure properties of large systems (e.g., long chain biomolecules) with few or no simplifying assumptions. Finally, the chronological thread delineated also provides the backdrop for asking counterfactual ("what if") questions examining, from a historical vantage point, the relative roles of computational power and theoretical intuition in the development of computational chemistry. Contrary to widespread notions that advances in computational chemistry are solely potentiated by increases in computing power, the article argues – via examples - that the relationship between theoretical imagination and computing power is more nuanced: specifically, the two alternately exert their influence at different junctures during the field's evolution.

Keywords: chemical bonding; modelling; atomic model; Schrodinger equation; approximate solutions; computational speed; intuition; imagination; science history;

PeerJ PrePrints | http://dx.doi.org/10.7287/peerj.preprints.365v1 | CC-BY 4.0 Open Access | received: 15 Apr 2014, published: 15 Apr 2014

Subject areas: biochemistry; bioengineering; computational science; computational biology; biophysics;

Conflict of Interest

The author declares no conflict of interest.

Author's contributions

Wenfa Ng wrote the paper.

Funding

No funding was obtained for this work.

PeerJ PrePrints | http://dx.doi.org/10.7287/peerj.preprints.365v1 | CC-BY 4.0 Open Access | received: 15 Apr 2014, published: 15 Apr 2014