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A Transition from Paper Pencil Scientist to Methodology Developer

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When is the last time you interacted with a paper-pencil scientist? The development of theoretical sciences, in particular theoretical chemistry has been interesting where paper pencil scientists used to be a dominating community. Many of earlier developed theories were based on fundamental scientific principles with use of cross disciplinary concepts. The endeavor of theory is to explain existing natural and experimental observations and provide prediction for their future behavior. Some of the important earlier developments in theoretical chemistry which can be considered as paper-pencil formalisms include Huckel theory, valence bond theory, molecular orbital theory, population analysis and evolution of Hartree-Fock as well as post Hartree-Fock methods like configuration interaction and much body perturbation theory. Many of these formalisms were amenable to computation. Thereafter, proposition of density functional theory (DFT) further changed the landscape of theoretical chemistry and attracted many budding scientists towards it. Prior to development of DFT, Thomas-Fermi model and Hartree-Fock-Slater method can be considered as paper-pencil formalism. Many of fundamental developments within density functional theory such as Hohenberg-Kohn theorem, Kohn-Sham formalism also can also be categorized here. Choice of paper pencil scientific career was natural for many theoretical chemists because very few researchers had computer facility. Such type of research required in-depth knowledge of multiple disciplines for proposition of newer theories. Therefore this career was usually chosen by those who had flair for Physics, Chemistry and Mathematics. This community used to be closely networked but faced significant criticism from colleagues in experimental Physics and Chemistry as it was difficult to demonstrate utility of proposed formalisms.

The paper pencil theoretical chemists could rarely demonstrate utility of proposed formalism in several chemical situations due to lack of widespread use of computers. With the availability of computers as well as software post-1980, the community of pure paper-pencil theoretical chemists reduced and community of researchers focusing on application of theoretical methods via computer software to solve meaningful chemical problems grew. The trend of choosing larger systems for investigation to check limits of theory and computation continues to attract significant interest of computational Chemists. Further, paper-pencil chemists did not make use of large amount of data to propose theoretical model but used fundamental principles available in the field of interest. Currently due to availability of data, several formalisms are proposed with use of data or theories are validated using this data. This change in the focus has been a good development for maturation of field since theories not only get proposed but also computer programs are written and tested for validation of proposed theory. Recently a completely new paradigm based on use and interpretation of chemical data has emerged which is broadly termed as cheminformatics (Data intensive or data oriented Science is also referred to as the 'Fourth paradigm' a vision pioneered by Jim Gray). Several graph theoretical descriptors used in Cheminformatics can be considered as paper-pencil formalisms.

With emergence of computer, the applied scientist community which uses existing algorithms to solve exciting problems has increased and is currently dominating most of the theoretical and computational chemistry. At present we see that 90% of work that gets published can be considered as computational chemistry rather than theoretical chemistry. Currently we see that prediction accuracy of theoretical and computational methods has reached to such level that it can challenge as well as guide experiments. However, we still need new concepts for improving existing theories in order to explain experiments and predict their future. This cannot be done only by paper-pencil scientist but requires transition of paper pencil scientist in to methodology developer. Methodology developer will generate concepts and formalisms, develop corresponding algorithms as well as computer codes and provide new way of interpretation of results thus obtained. Once such methodology is developed and is sufficiently exciting, application scientists will pick this and apply it in different areas to identify strengths and limitations of proposed methodology. One such early example of transition of paper pencil formalism to methodology development can be seen in Extended Huckel Method (considered as mother of all semiempirical methods) developed by Roald Hoffmann.

Hoffmann went through all phases of methodology development like formalism proposition, algorithm development and extensive application of this method. We need to consciously be aware that we need good balance of both the communities, viz. methodology developer and application scientists for progress of theoretical and computational chemistry. A methodology developer will now replace paper-pencil scientist from past.

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