

COMPUTATIONAL CHEMISTRY'S EVOLUTION, FROM ANALOGUE TO DIGITAL, ENHANCES RESEARCH ACROSS DISCIPLINES WITH PROMISING AI AND QUANTUM INTEGRATION

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Abstract

Computational chemistry is an inter-disciplinary field, which has been modified tremendously with the support of internet computing to study chemical processes. This paper presents a short summary, showing how it came along from analog to digital computers and pointing out the main discoveries of pioneers. It describes various approaches such as quantum mechanics, molecular dynamics or spectroscopic simulations that are employed to analyze the behavior of molecules. The field of computational chemistry has had very significant impacts in drug discovery, materials science environmental chemistry and biology. However, computational cost and accuracy remain as challenges. However, the future is filled with an optimistic outlook due to AI integration and quantum computing within interdisciplinary cooperation that broadens the scope of its capabilities and scientific.

Keywords: Computational Chemistry, Historical Perspective, Digital Computing, Quantum Mechanics, Molecular Dynamics, Spectroscopic Simulations, Drug Discovery, Materials Science, Environmental Chemistry, Biological Systems, Pioneers, Ab Initio Methods, Density Functional Theory, Machine Learning, Quantum Computing, Interdisciplinary Collaboration, Challenges, Future Prospects, Scientific Discovery, Technological Advancement.

INTRODUCTION

Computational chemistry is a science that combines several scientific fields and makes use of the computer simulation to help solve some chemical problems. It implements the approaches of theoretical chemistry, implemented in effective computer programs, to calculate the forms and characteristics of molecules and solids. This area plays a critical role in many areas such as drug design, material synthesis, and fundamental chemistry. Computational chemistry, which has a wide range of methods that are constantly changing, is an important aspect in the study of molecular behaviour and chemical processes. It supplements experimental chemistry, gives a perspective that is not available from experiments alone and provides for the design and prediction of novel chemical entities and materials. With increasing computational power and the development of new methods, computational chemistry will continue to provide even more important contributions to science and technology (Adams & Sonntag, 2018).

The history of computational chemistry is an interesting journey that represents the synthesis of mathematics, physics and computer science in order to unravel the mystery behind chemical processes. The first mention of the utilization of computers, analogue ones at that time, to solve complex chemical issues dates back to the mid-20th century when scientists became aware of this potential. The first attempts focused on using these analogue machines for calculations related to quantum mechanics and molecular structure, which laid the groundwork of computational chemistry in their infancy (Ballentine, 2014). But the real revolution occurred with digital computers introduced in 1940s and 1950s. These digital machines signified a change in paradigm, freeing the scientist from analogue computing. This computing revolution enabled researchers to carry out numerical computations for chemical systems with impeccable accuracy and high speed (Bronstein, 2003). The trend for the 1950s and the early sixties was in interest of computational method, which tried to mimic quantum mechanical solutions molecules or chemical reactions. Among the primitive attempts were Hartree-Fock methods as a means of reference for electronic structure calculations. It is at this point that the discipline of computational chemistry emerged. The first quantum chemistry programs appeared in the 1960s. The contributions of visionary scientists namely John Pople and Roald Hoffmann were enormous as they created computational methods and software to do the electronic structure calculations on models. This was a turning point in the field's development, allowing researchers to investigate the electronic properties of molecules with unparalleled detail (Drews, 2000; Callister Jr. & Rethwisch, 2020). At the same time, molecular mechanics was developed in the 1960s and 1970s. Molecular mechanics was the first one to propose using simplified models based on empirical force fields to explain molecular interactions. This method was especially useful in the study of large molecules and materials, pioneering new fields in biology and materials science (Feller, 1996). The growth of computational chemistry led to the increase in its applications. It was of great importance in the 1980s and 1990s for drug discovery, reaction mechanism studies, catalysis, and materials science. This made the researchers to depend on computational methods for predicting molecular properties thus leading to new developments in the field (Edelman & Gally, 2001). Progress in the field of theoretical studies resulted in the creation of more precise tools with density functional theory (DFT) becoming a standard episteme at the end of 20th century. Despite their high computational cost, *ab initio* methods began to provide very accurate results and were widely adopted. The late twentieth century was the supercomputing period as powerful machines became available that could handle complex problems, simulate larger systems, and investigate chemical reactions in longer time scales. During this time, the new era of computational power came which facilitated researchers in analyzing data more complicated research issues (Goh et al., 2017). Therefore, it is a considerable part of the modern scientific era represented by computational chemistry. It promotes interdisciplinary research, combining chemists and physicists, biologists and materials scientists to solve difficult problems. Computational approaches have applications across a wide variety of fields such as drug

design, materials discovery, environmental chemistry and bioinformatics (Gombar et al., 2007). Looking to the future, computational chemistry has a bright future. Quantum computing has been in the limelight due to its ability of computerizing mathematical formulas and models, which is bound to transform how quantum systems are presented. In computational workflows, machine learning and artificial intelligence are being blended unimpededly into the same stream accessing efficiency to increase the predictive power. The multiscale modelling approaches will fill the gap between different levels of chemical systems and also unify complex phenomena (Hoffmann et al., 2020). It implies that the historical perspective of computational chemistry highlights that the huge voyage of computing capacity to open up science secrets, which are covered by. Computational chemistry has evolved from the humble start with analogue computers to supercomputing and interdisciplinary cooperation that will continue shaping our knowledge of chemical processes and steering science advanced technology (Hollingsworth & Dror, 2018).

Table 1*Historical perspective of Computational chemistry*

Time Period	Key Developments
Mid-20th Century	Recognition of analog computers for chemical calculations
1940s - 1950s	Advent of digital computers for chemical simulations
1950s - 1960s	Development of quantum mechanical methods like Hartree-Fock
1960s	Emergence of first quantum chemistry programs
1960s - 1970s	Introduction of molecular mechanics
1980s - 1990s	Computational chemistry's role in drug discovery and materials science
Late 20th Century	Rise of supercomputing for complex simulations
Modern Era	Integration into interdisciplinary research
Future Prospects	Advances in quantum computing and machine learning

2. METHODS

Theories advanced, and more accurate methods emerged as density functional theory (DFT) became a base for the late 20th century. The ab initio approach, although computational expensive, started providing extremely accurate results that attracted broad acceptance. The late twentieth century was the time of supercomputers as powerful machines were readily available to handle complicated problems, simulate larger systems and explore chemical processes over a longer period of time. In this time such a new wave of computing power to generate emerged that presented further, the case for researchers to investigate yet more critical study questions (Goh et al., 2017).

Computational chemistry is one significant part of the contemporary scientific age. It promotes interdisciplinary partnership, uniting chemists and physicists, biologists and materials scientists to solve multiple problems. Computational approaches have applications across a wide variety of fields such as drug design, materials discovery, environmental chemistry and bioinformatics (Gombar et al., 2007).

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Another significant technique is the Monte Carlo Simulation, which provides a special focus on systems with many interacting degrees of freedom called liquids and disordered materials. This approach involves various simulations that are based on the use of a certain form of random sampling, and it is characterized by its versatility (Young, 2004). Computational chemistry covers the spectroscopic simulations of NMR, IR, UV-vis and EPR types that are used for better understanding these spectra. This is essential as vibrational spectroscopy methods simulate both IR and Raman spectra, with supplemental means to understand molecular motions and effects. At the same time, computational approaches including Docking and Pharmacophore Modeling play a fundamental role in discoveries of various drugs used by the pharmaceutical industry. Docking predicts the orientation and binding of molecules, such as drugs to their targets while pharmacophore modeling identifies a group arrangement necessary for interaction with biological target (Mahato & Pramanicka 2015b). To this end, transition state theory (TST) uses both qualitative and quantitative methodologies to determine the specifics of these reactions through describing their outcomes, entropies, as well as energies. It allows to judge reaction kinetics and take a closer look at thermodynamics.

Computational Chemistry Software

There are many computer packages that can be used to carry out these calculations; for example, Gaussian, GAMESS NWChem VASP Amber gromacs and many

others. These types of software tools offer a variety of functionalities and are selected in accordance with the actual research goals and reflecting on systems being investigated (Edelman & Gally, 2001).

Table 2*Computational Chemistry Methods and Tools*

Category	Method/Tool	Description	Applications
Quantum Mechanical Methods	Hartree-Fock (HF), Post-Hartree-Fock, Density Functional Theory (DFT)	Accurate, based on quantum mechanics, computationally demanding. DFT balances accuracy and efficiency.	Detailed electronic structure studies
Semi-Empirical and Empirical Methods	AM1, PM3, MNDO	Approximate electronic wave function, use empirical parameters.	Larger systems where full quantum methods are impractical.
Molecular Mechanics (MM)	Classical physics principles	Treats atoms as spheres, bonds as springs	Ideal for large biological molecules.
Molecular Dynamics (MD)	Simulation of physical movements	Simulates atoms and molecules over time	Protein folding, diffusion, chemical reactions in solutions.
QM/MM Hybrid Methods	Quantum Mechanics/Molecular Mechanics	Combines quantum mechanics for reactive parts and MM for the rest.	Chemical reactions in biological systems.
Monte Carlo Simulations	Random sampling techniques	Used for systems with many coupled degrees of freedom	Studies of liquids, disordered materials
Spectroscopic Simulations	Vibrational Spectroscopy Methods	Simulates vibrational spectra (IR, Raman).	Interpretation of NMR, IR, UV-Vis, EPR spectra; understanding molecular interactions.
Drug Discovery	Docking, Pharmacophore Modeling	Docking for molecule orientation and binding, pharmacophore modeling for identifying structural features.	Predicting drug-target interactions, structural features for biological targeting.
Reaction Studies	Transition State Theory (TST)	Identifies transition states and reaction pathways.	Insights into reaction kinetics and thermodynamics.
Computational Chemistry Software	Gaussian, GAMESS, NWChem, VASP, Amber, GROMACS, etc.	Various software for different computational chemistry calculations.	Depending on research objectives and system studied

3. RESULTS

Computational chemistry has led to groundbreaking discoveries in both scientific and industrial areas. This interdisciplinary field typically combines concepts of chemistry, physics, and computer science for the study on molecular behavior prediction properties to enable discovery new molecules or materials. In this section, we discuss the main outcomes and gains from computational chemistry across various areas of usage (Bronstein, 2003).

Drug Discovery and Development

Calculations in the field of computational chemistry have a central role to play when it comes to potential drug discovery, significantly accelerating finding candidate drugs. By using molecular modeling and virtual screening, it is possible to filter through thousands of compounds based on their binding affinity towards a given drug target such as proteins or enzymes. These have resulted to the identification of various drugs such as antiviral medicines, cancer medications and antibiotics (Young, 2004).

A famous case in point is the development of ritonavir, an HIV protease inhibitor. This drug was designed with the help of computational means that in turn popularized treatment of HIV/AIDS by blocking its replication. Analogously, in drug development for new antibiotics, computational chemistry helps to achieve the goal of identifying compounds that attack bacterial enzymes but spare human proteins – an important challenge is posed by antibiotic resistance (Maginn & Elliott 2010).

Materials Science and Engineering

Computational chemistry has brought a new revolution towards materials science through giving insights on the properties and behavior of substances at atomic to molecular level. This information allows the creation of highly developed materials with conditional properties for different uses. Applications of computational chemistry in the catalysis sector have played a valuable role by designing highly efficient catalysts for chemical reactions, thereby promoting sustainability and energy conservation. Computational methods have also been used by researchers to find catalysts that Aid in hydrogen production and carbon capture among other processes (Lewars, 2011).

In addition, at the level of semiconductors and nanomaterials computational chemistry has helped progress towards next-generation electronics storage devices. For instance, the elucidation of novel organic semiconductors and battery materials has been made possible thanks to predicting their electronic properties and stability through simulations (Leszczynski 2012).

Environmental Chemistry

Toxicity of different chemical compounds and pollutants may be assessed by computational chemistry. With the help of predictive models, researchers can understand how those pollutants are dispersed in air, water and soil. This information is useful in the development of safe and green chemicals as well procedures (Ballentine, 2014).

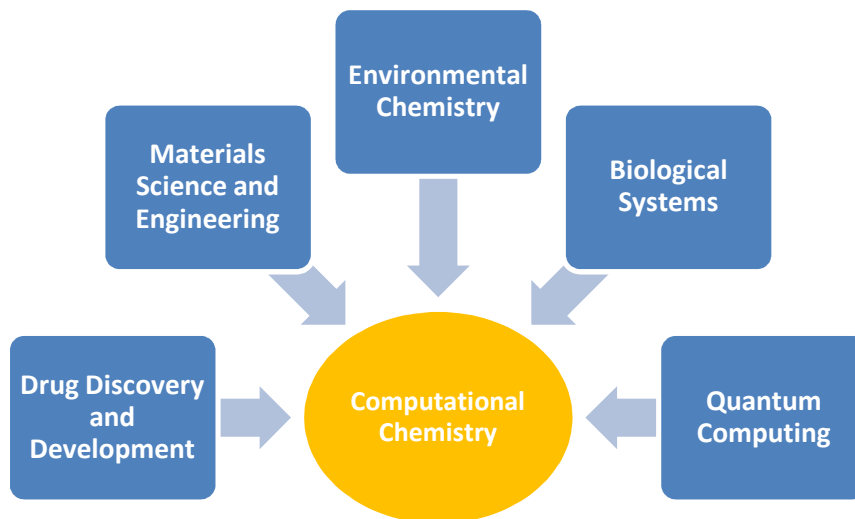
One of the contribution was made in hydrocarbon s and climate change. Computational chemistry has contributed to the understanding of mechanisms responsible for greenhouse gas absorption and emission that have been essential in climate modeling as well as facilitated evolution of various strategies used in attempts aimed at minimizing global warming. Moreover, the development of efficient sorbents for the absorption of CO₂ from industrial effluent largely depends on computation simulations (Morzan et al., 2018).

Understanding Biological Systems

Computational chemistry is essential to understanding complicated biological processes. One of the prime examples is reaction in proteins and nuclei acid by using molecular dynamics simulations through which one can develop a better understanding for dynamic behavior. This is indeed crucial for drug design and an appreciation of diseases at a molecular level. In structural biology, computational methods have supported the prediction of protein structures theoretically to X-ray crystallography and NMR spectroscopy. Computational chemistry played a pivotal role that materialized in the prediction of SARS-CoV2 spike protein structure, leading to rapid development of COVID 19 vaccines (Miller et al., 2019).

Quantum Computing and Computational Chemistry

The computer technology will also further advance if quantum computational chemistry can be achieved for use in the field. Quantum computers offer accurate simulations of quantum systems, helping scientists implement molecular applications that were virtually impossible due to the computational burden. Some quantum algorithms such as the Variational Quantum Eigensolver (VQE) are being created to solve challenging molecular problems with an entirely unparalleled development speed and accuracy (Callister Jr. & Rethwisch, 2019). Hence, the progress of computational chemistry has become a permanent element in scientific research and production. Its involvement in drug discovery, materials science and environmentally safe buildings along with its impact on our environmental protection aspects are monumental. However, as the computer power continues to increase and new techniques are invented, computational chemistry will still be at a cutting edge of science and technology. It is a dynamic discipline that constantly challenges the limits of what can be achieved, opening new frontiers in chemistry and beyond (Pakkiraiah & Satyanarayana, 2023).

Figure 1: Results of computational chemistry

4. DISCUSSION

Computational chemistry is an evolving and multidisciplinary area that integrates the knowledge of principles underlying the chemical nature with elements from physics together with computer science to investigate as well as understand how matters occur at a molecular/atomic level. In this talk, we are going to discuss the pedigree of computational chemistry in further detail including its significance, obstacles and other future prospects (Feller, 1996; Drews, 2000).

Challenges in Computational Chemistry

Despite its strength, computational chemistry has many challenging problems both scientific and technical. Among the foremost problems is computational cost. Producing accurate simulations generally requires large computational resources. Naturally *ab initio* methods, having high reputation for accuracy are computationally intensive which limits their use to smaller systems. The methods of dealing with the discussed challenge also involve continuous algorithm optimization and use-up high computing performance infrastructure (Edelman & Gally, 2001; Bronstein, 2003). An ongoing trade-off between accuracy and computational efficiency. The results of researchers' research goals are judiciously chosen, both on the level and type of theory as well as approximation procedures. The issue of achieving an ideal compromise between precision and cost is important to being able to do meaningful simulations (Young, 2004; Maginn & Elliott, 2010). The other obstacle is the parameterization, which applies especially in molecular mechanics and semi-empirical methods. It is necessary to ensure that the accurate force fields and parameters are exactly calibrated

with experimental data. This development of parameterization for new molecules and materials is a very laborious process that takes up significant time, which restricts the research ground (Leszczynski 2012; Ballentine, p.37). The accurate modelling of such solvent effects is a daunting challenge to computational chemistry. The solvents play a significant part of chemical reactions and molecular interactions. However, although implicit solvent models are fast and computationally efficient they do not provide the accuracy that is required for some studies. However, explicit solvent models provide for higher accuracy but are computationally costly thus offering a dilemma between efficiency and precision (Goh et al., 2017; Hollingsworth & Dror, 2018). Simulating chemical processes that occur over the long time scales exists another challenge when we are talking about protein folding or complex and non-linear chemistry reactions. In order to address this shortcoming, improved sampling techniques and approximations are undertaken for enhancing researchers with other views into complicated processes (Miller et al., 2019). More notably is the emerging opportunity for a new and unique way that this computational chemistry may adopt quantum computing. Quantum computing is the field of immense possibilities pertaining to many complex quantum mechanical equations with high efficiency. Quantum algorithms are also in the development pace to solve an even complicated molecule problem which opens new vistas for further researches (Callister Jr. & Rethwisch, 2020).

Future Prospects

The future of computer chemistry is full to the brim with opportunities and inventions. In this manner, the application of machine learning and AI is poised to revolutionize credentials in these fields. Such tools are useful for rapid orientation, prediction of chemical properties and process automation in new molecule and material discovery. AI-driven methodologies have already garnered significant leverage in the field of drug discovery and materials designing, making sublime research and experimentation easy (Morzan et al., 2018). A quantum revolution like that brought by computational chemistry is one example in the field of Computation Chemistry. Capability of modelling the quantum systems to achieve absolute precision that cannot be compared with anyone else and speeds allows it advance into no man's land of research. Quantum algorithms are now coming up, which can predict breakthrough findings with respect to solving complex molecular problems (Hoffmann et al., 2020).

Multistage modelling progress helps to overcome the link between various levels of chemical systems. The holistic nature of the approach enables researchers to study phenomena that are both large in scale and long lasting, improving our understanding of chemical processes. Combining computational chemistry with chemo informatics; additionally employing big data analysis not only assists scientists discover entirely new molecules and materials but also fosters development within various economic sectors.

Prior screening and identification of potential candidates become far easier with the help of large databases holding all possible chemical information, which also promotes a faster research process (McArdle et al., 2020). Interdisciplinary is here to stay. Joint ventures across computational chemistry and the like biology, materials science as well environmental research are anticipated that will produce solutions to complex challenges. This multi – disciplinary framework will help to expand the use of computational chemistry in various fields (Gombar et al., 2007).

Education and training programs are essential to endow the following generation of researchers with skills and knowledge in order for them solve computational chemistry's power. The speed at which the field is advancing will require a knowledge and well-trained workforce who have been trained to leverage its potential for progress towards scientific discoveries and renewed technological advancements (Pakkiraiah & Satyanarayana, 2023).

Table 3*Challenges and future prospects*

Aspect	Challenges	Future Prospects
Computational Cost	Extensive computational resources required for high accuracy Limitation of ab initio methods	Optimization and utilization of high-performance computing Integration of quantum computing
Accuracy vs. Efficiency	Balancing precision and computational efficiency Selection of appropriate methods	Integration of machine learning and AI to enhance efficiency Development of quantum algorithms
Parameterization	Time-consuming calibration of force fields and parameters	Advancements in automated parameterization Use of large chemical databases
Solvent Effects	Complex modeling of solvent influence on reactions	Development of more accurate solvent models Advancements in hybrid quantum-classical methods
Time Scales	Challenges in simulating long time-scale processes	Enhanced sampling techniques and approximations Multiscale modeling
Quantum Computing Integration	- Quantum computing in its early stages	Full integration of quantum computing into workflows Quantum algorithms for complex problems

CONCLUSION

Finally, computational chemistry is a fast moving and essential science that link up chemistries as well as physics researchers along with their counterparts in computer sciences. Its historical evolution from analogue to digital computing has given scientists the ability of disclosing chemical phenomena with microscopic accuracy. Record figures

such as John Pople and Roald Hoffmann have acted as forerunners in the development of various approaches that has ranged from quantum mechanics to molecular dynamics, enabling us comfortable examination on how molecules behave. The number of influences the computational chemistry has in drug discovery, materials science, environmental chemicals and biology speaks by itself. It has greatly shortened the process of locating essential drugs, improved catalyst design, helped the generation and modernization of materials used in industrial processes as well as contributed to environmental science and biological systems. Despite the ongoing challenges, such as computational cost and accuracy vs. efficiency balance, it remains an area that is able to develop exponentially in future; especially with rising demand from renewable technologies for chemical components. Combining with AI and quantum computing alongside interdisciplinary cooperation as well as rigorous education and training programs certainly, will accelerate this area to even further stunning scientific expeditions of breakthroughs together technological innovations. The continued advancement of computational chemistry carves out unexplored and passages in the domain of chemical reactions, as well as beyond.

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