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Commentary

Correlation Techniques for Computational Science and Engineering by using Machine Learning

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DESCRIPTION

We have witnessed unprecedented advancements in scientific research and discoveries over the past half century. The exponential technological evolution is undeniable, with breakthroughs in everything from fundamental physics, like particle physics, to engineering applications, like biomedicine, electronics, and materials science. The fundamental laws that govern our universe are laid out in theoretical physics in the form of partial differential equations, and analytical solutions to all but the most trivial problems are impossible. Computer simulations that numerically solve these equations are needed to solve the aforementioned problems and help optimize engineering solutions. However, computational modelling does not yet meet expectations. Many contemporary physical problems, typically those involving phenomena at multiple length and time scales, require computational resources that are quickly becoming prohibitive. The most fundamental theory to date is known as Quantum Mechanical (QM) Density Functional Theory (DFT) and other quantum mechanical simulations are practically limited to a small number of atoms, making them useless for the majority of engineering issues. Instead, using Newton's second law of motion, Molecular Dynamics (MD) simulations simulate atomic trajectories and continuously update the system. Systems with characteristic dimensions of the nanometer to the micrometer, such as micro and Nano fluidics and numerous chemical applications are frequently studied using MD. Particle interactions are governed by semi-empirical models derived typically from QM data. However, while they may be accurate for particular thermodynamic states and properties, they may not always be applicable to other conditions or properties. In addition, covalent bonds frequently have a fixed and explicit pre-defined nature. In this way, compound responses are not intrinsically caught by MD and explicit models, for example, Receptive Power Fields. QM and particle-based approaches can only describe a small portion of engineering issues. The molecular structure of a system in continuous-based physics like fluid dynamics, which instead focus on averaged properties like density, pressure, and velocity as they change over time and space. The cost of computing is significantly reduced as a result. Using a grid, simulation techniques like Computational Fluid Dynamics (CFD) divide up space. The accuracy improves with grid density, but at the expense of computational cost. Aerospace, automotive, and biomedical industries have all benefited from these methods. And these Menthods focus on specific industrial applications or physics fields to address the numerical and physical challenges. Additionally, despite significant advancements in the field, a number of issues remain unsolved. Turbulence, a flow regime characterized by fluctuations in velocity and pressure, instabilities, and rotating fluid structures known as eddies that appear at various scales, from vast, macroscopic distances to molecular lengths, is perhaps the most important example. A large number of grid points are required for a precise CFD description of the physics of transient flows. Direct Navie Stokes (DNS) is a method in which the Navier–Stokes equations are directly applied, but it comes with a significant computational cost. As a result, it can only be used to solve specific problems, necessitates extensive High Performance Computing (HPC) facilities, and has extremely long run times. The accuracy of reduced turbulent models is frequently sacrificed in their use. In addition, even though there are a lot of these methods, there is no one-size-fits-all model that applies to all turbulent flows. Finding a good balance between accuracy and computational resources is a crucial objective in computational modelling and simulation. For instance, QM-based simulations could be used to accurately resolve complex, turbulent flows if there were no computational limitations; However, in practice, this is an impossible task. We present ML-based research with the goal of achieving a better balance between speed and accuracy in this section. Recreation strategy that settle the framework down to the nuclear scale. MD is based on physics from Newton. A single point represents each atom. It is disregarded its electronic structure, whose dynamics are described by QM. The gradient is used to calculate the forces acting on the particles. Additionally, data mining and processing benefit greatly from ML. Biomedicine, for example, has taken advantage of these technologies by employing more sophisticated algorithms to illuminate the vast and intricate data required by these fields. However, we do believe that employing such strategies can have a significant impact on other sectors. Transitional and turbulent

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flows are two examples, where massive DNS simulations reveal temporary structures that are often too complex to comprehend through conventional methods or visual inspection. These kinds of structures can be categorized and correlations can be found using ML algorithms. Microscopic simulations are similar. Machine Learning (ML) algorithms are quickly spreading to practically every scientific field. This article provides a brief summary of some of the most recent efforts and developments utilizing ML in science and engineering. We believe that despite its enormous success in recent years, Machine Learning (ML) is still in its infancy and will have a significant impact on engineering and scientific research in the coming years.