Commentary

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The Molecular Graphics and Modelling Society

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Description

The Journal of Molecular Graphics and Modeling, formerly known as the Journal of Molecular Graphics, is the subject of this bibliometric review. Since its inception in 1983, the journal has seen rapid expansion, with articles coming from all over the world. Instead of focusing on the underlying technology that was the focus of many of the early papers in the journal, it now primarily contains articles that describe applications of molecular graphics and modeling in chemical and biological systems; However, the earliest system-based papers continue to receive the greatest number of citations.

Evolved Into Molecular Graphics Society and MGMS

The Journal of Molecular Graphics which later evolved into the present-day Journal of Molecular Graphics and Modeling was founded by the Molecular Graphics and Modelling Society (MGMS).This brief article will provide a brief overview of the UK Molecular Graphics Group, which later evolved into the Molecular Graphics Society and then the MGMS, based on the MGMS archives. We cover the time between November 17, 1981, and the first annual general meeting of the Group on April 14, 1983.According to Prof. Graham Richards's article in this issue; it was during this time that the need for a new journal focusing on the emerging field of molecular graphics was recognized. Today, the MGMS is a successful society that organizes a variety of meetings, awards, lecture tours, bursaries, and other events to support education and research in molecular graphics and modeling. Drug design is one area where molecular graphics and modeling are now essential and integrated tools. However, the Society was founded forty years ago, before computers were widely used in scientific research and the visualization of molecules. The UK Molecular Graphics Group was the precursor to the MGMS, as previously mentioned. The Group's goal was the "formation of an energetic group that will benefit all its members," according to the initial invitation letter to its inaugural conference from November 17, 1981.As acting secretary of the Group, Andy Morffew of IBM organized this meeting, which was abbreviated to UKMGG; This meeting was a continuation of the initial informal gathering he convened in September 1981 at Balls Park to investigate the concept, as detailed in Prof. Richards' article in this issue. The Group was very successful in realizing this goal, as will become evident from the very active program of activities it had during its first year and a half, to the point where it was presented as the Molecular Graphics Society at its first Annual General Meeting in 1983. The Chairman's report from this AGM can be found in the minutes: "The MGS has been in existence for nineteen months since the first seeds were sown in September 1981."It started out as the United Kingdom Molecular Graphics Group, but its reputation in Europe and the United States as the only organization dedicated solely to molecular graphics issues has greatly expanded. In the 1980s, the term "molecular graphics" had a slightly different meaning than it did in later years, encompassing not only visualization and graphics techniques but also the use of molecular calculations to solve problems in chemistry and biology. At this point in time, the definition implied that modeling and graphics were included as well. In the 1990s, the Society and the Journal explicitly acknowledged modeling by including the term "modeling" in their titles.

Significant Development in Scientific Computing

The introduction of the Compute Unified Device Architecture a parallel computing platform and application programming interface model developed by NVIDIA Corporation, has been a significant development in scientific computing in recent years. When compared to CPU-based implementations, CUDA speeds up scientific computing by tens to hundreds of times. Researchers and engineers can take advantage of the massive computing power provided by the thousands of computing cores on NVIDIA GPUs. OpenCL is another structure that supports equal programming for GPU and empowers universally useful registering on GPUs from different merchants. Many MD codes, including LAMMPS, AMBER and Gromacs now offer options for transferring the parts of the code that require a lot of computation to the GPU at each time step. A number of MD codes, such as RUMD, OpenMM, crystal MD, ACEMD, HAL's MD, and HOOMD-Blue, have been developed from the ground up to utilize the full computational power of GPU by implementing the computing process entirely on GPU. This is done in order to avoid the inefficient back-and-forth transferring of data between the host and the device. These GPU implementations of MD all focused on increasing computational speed for small to

medium-sized systems on a single GPU, i.e. systems with thousands to a few millions of atoms, and resorted to multiple GPU systems, such as computer clusters for handling systems with more atoms. This is a common feature of these GPU implementations of MD. What is less examined is the MD reenactment of enormous scope frameworks on a solitary GPU, for example frameworks with a huge number of molecules. This makes it difficult for many engineers and researchers who don't have access to supercomputers to investigate problems that require MD simulation at a modeling scale of several tens to hundreds of nanometers. Ultra-precision machining, atomic force microscopy, and nano electro-mechanical systems, all of which involve extensive deformation on the order of several tens to approximately one hundred nanometers, are examples. Experimentation and continuum methods like the finite element method make it challenging to model phenomena on this scale. Although MD is the best approach for modeling phenomena on this scale, its use is severely constrained by the high cost of supercomputers.