Editorial

In the Notes for Authors we state that "the journal is devoted to the publication of high-quality practical and theoretical papers on the use of computer graphics for the investigation of molecular structure, function and interaction." However, to display results we first have to produce results, and one of the fastest growing ways to do that is through the use of Artificial Intelligence (AI). With that in mind, the editors decided that we would publish a special AI issue as a service to our readers, even though the papers would not be heavily oriented toward graphics.

Trying to precisely define AI is a little like trying to put a pin through a blob of mercury; the job is difficult, the task is constantly shifting, and it's not clear that once you have finished the job that you will have achieved a permanent and useful goal. So I will loosely define AI as programming that primarily utilizes symbolic knowledge and logic as opposed to numerical programming. This allows us to broadly separate the more numerically based programs (such as an Ab Initio Quantum Mechanics program) from symbolic programs (such as Expert Systems), even though the former certainly utilize logical flow of control and the latter often use some math.

Certain tasks are more ideally suited for solution by symbolic manipulation than by utilizing a numerical algorithm. This can either be due to the symbolic nature of the problem, or in those cases where no numerical solution has yet been defined. Theorem proving is an example of a case that is obviously both logical and symbolic in nature, as is a chess game. Planning an organic synthesis or determining the metabolic fate of a drug can be likened to a chess game. The states are described by naming the individual pieces and their positions. These logical descriptions are then used to ascertain interactions between pieces. Logical rules are then applied to decide what state transformations are possible and/or desirable. The total number of all possible states is so large that no program could ever hope to examine them all, so intelligent guesses (heuristics) must be applied to help us find the best or most probable paths. The area of AI research called Vision Understanding is another area where logical reasoning based on symbolic analysis has made great strides, and those lessons can be applied to chemistry.

This issue contains four invited papers that deal with these topics. This issue cannot cover the broad range of work being done in the application of AI to chemistry, as that would require a weighty tome. Instead, we hope that by presenting some highlights we will whet your appetite for more. With the advent of AI workstations that contain high quality graphics, it is certain that we will soon be seeing a tighter coupling of AI and graphics appearing in this journal. I, for one, look forward to these new developments.

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Special Issue Editor