

ATOMIC SCALE MODELING OF POLYMERIZATION CATALYSTS

Developing new forms of plastic and improving the efficiency of the catalysts that produce them requires detailed insight into the reaction steps in the polymerization process. This calls for thorough analysis and hefty computational resources. The authors discuss their strategies for accurate modeling and Cobalt—a Beowulf supercomputer they built and optimized for quantum chemistry applications.

Plastic is a ubiquitous material in modern society. Indeed, industry manufactures hundreds of billions of kilograms of plastic each year. Grocery bags, packaging, UV-resistant car interiors, fibers for clothing, medical tubing, and other sterile medical devices are a few examples of the broad range of products made from plastic.

This incredible breadth results from the ability to engineer a wide range of physical properties. Thus, catalytic processes are becoming increasingly important in the industrial production of plastics. A polymerization *catalyst* is a molecule that joins monomer units continuously to form a long chain, or *polymer* (see Figure 1). The catalyst's molecular architecture governs the elementary reaction steps that control the polymer's nature. When examined at the atomic level, the catalyst is a molecular-sized machine that assembles the polymer monomer-by-monomer at breakneck speeds

(typically on the order of thousands per second).

At the University of Calgary, we developed computational modeling strategies and the supercomputing capability required to accurately model catalysis used in the production of plastics. Our modeling strategy makes uncovering the details of the catalyst's architecture and reaction steps possible, expanding the chemist's ability to rationally engineer new catalysts and, potentially, new plastics. With *Cobalt* (computers on benches all linked together), the Beowulf supercomputer we built, the computing resources required to execute our modeling strategy are within the reach of even small research groups with limited budgets.

The industrial production of plastics

Approximately 85% of the thermoplastics produced each year are *polyolefins*, plastics made from a chemical unit called an *olefin* (a molecule with a carbon-carbon double bond). Well-known examples of polyolefins include polyethylene, polypropylene, and polystyrene. Our research focuses on studying the key elementary reaction steps of the catalytic processes. The ultimate goal of the research is to use this detailed knowledge to rationally improve and design new and better catalyst architectures.

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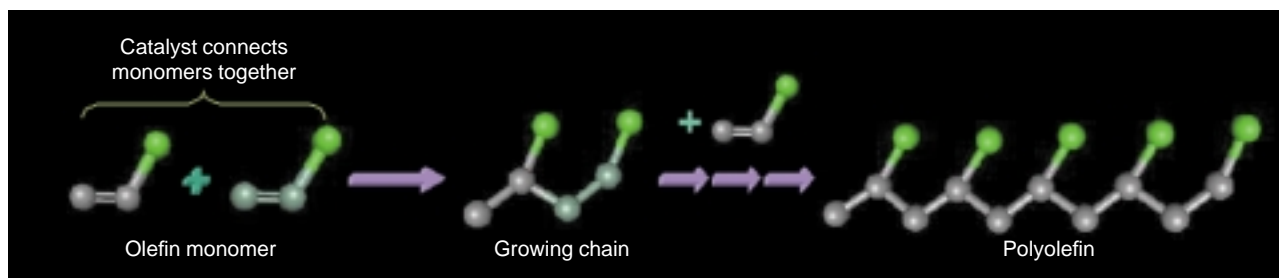


Figure 1. The catalyst acts as a molecular machine by joining the monomer molecules together in rapid succession.

The original catalyst

Most manufacturing processes for polyolefins use a catalyst-based process that originated from the 1950's Nobel Prize winning work of Karl Ziegler and Giulio Natta. Despite their importance, the Ziegler–Natta catalysts offer only limited control over the range of polymer properties produced. Part of the problem is that the catalyst's structure remains elusive, making it difficult to rationally improve the catalyst. Consequently, any improvements to Ziegler–Natta catalysts are, for the most part, the result of trial-and-error experimentation.

New-generation catalysts

In the early 1980s, single-site catalysts began to revolutionize the industrial production of polyolefins.^{1,2} The fundamental difference between these single-site catalysts and the Ziegler–Natta catalysts is that single-site catalysts have a well-defined molecular structure. These new-generation single-site catalysts promise to be more cost-effective, and more importantly, they expand the range of plastics produced on an industrial scale. Several never-before-made classes of plastics are a result of single-site catalysts.

Because the structures of the single-site catalysts are well defined, they enable some degree of rational catalyst engineering. In some cases, the relationship between the catalyst structure and the resulting plastic is clear. Figures 2a and 2b demonstrate two classic examples of this. The left-hand side of the figure depicts the catalyst systems designed to produce the desired polymer structure. In these cases, the chemists made key assumptions concerning the elementary reaction steps involved in the catalytic cycle. With these assumptions, it is evident that the catalyst structure's symmetry controlled the placement of the monomer substituents (depicted in green; see the right-hand side of Figures 2a and 2b).

However, as the molecular architecture's complexity increases, the relationship between the

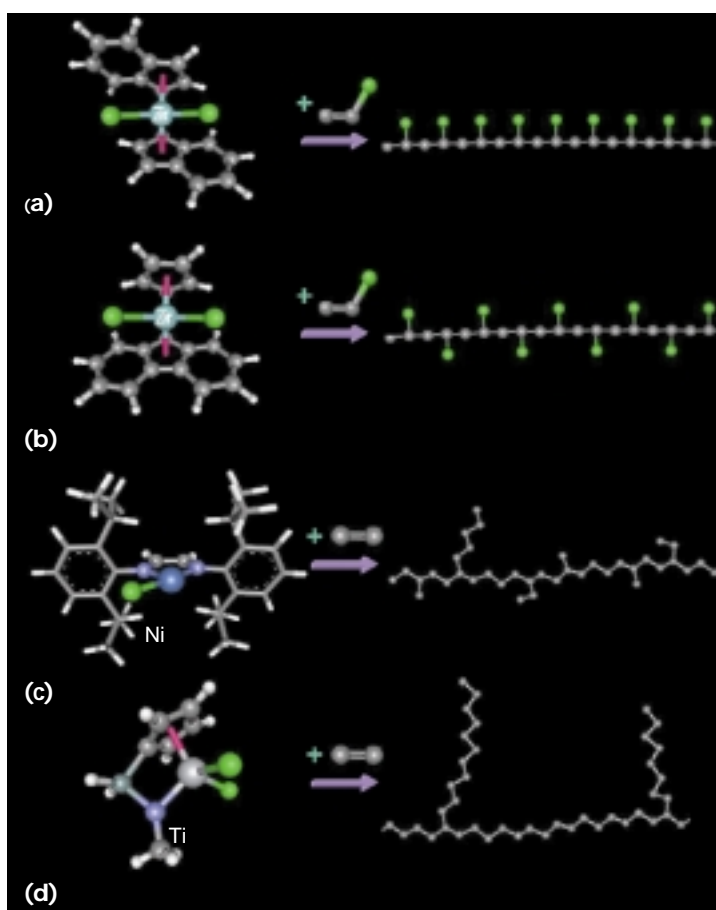


Figure 2. Examples of single-site catalysts with representations of the corresponding polymers they produce. Catalyst (a) produces a polymer with side chains (shown in green) with the same orientation. Catalyst (b), on the other hand, produces polymers with side chains that alternate their orientation. The catalyst in (c) produces a polymer with numerous short side chains even though the monomer has no side chains. Catalyst (d) produces a polymer with a few long side chains even though the monomer has no side chains.

catalyst structure and the resulting polymer structure is not as obvious. Figures 2c and 2d provide examples where the resulting polymer has side chains although the monomer does not. Although the chemist might know the single-site

catalyst's structure, the details regarding the elementary reaction steps—the information that is important to control the final polymer's structure—is still unknown. Therefore, many improvements to the single-site catalysts result from trial and error as well.

Improving the process through computational modeling

At best, experimentally probing the details of elementary reaction steps is exhausting and difficult work. Here, computational modeling is a valuable tool. Computational modeling allows an atomic-level examination of the catalytic cycle's elementary reaction steps. This provides a deep, fundamental understanding of how the catalysts operate, which ultimately provides the basis for rational catalyst engineering and further technological innovations in the plastics industry.

The foundation

The calculation of the *potential energy surface* is the foundation of the computational modeling techniques we use. The PES is the hypersurface that relates the molecular system's geometry to the system's total energy. Predicting or understanding the resulting polymer's nature requires full knowledge of the PES for each of the catalytic cycle's elementary reaction steps.

For example, the PES's topology governs how much of a hill or barrier there is to each elementary reaction step and whether the process is thermodynamically favorable. An efficient catalyst should have a small barrier to the reaction step or steps that grow the polymer chain. A good catalyst should also have a relatively high barrier to the process that stops the polymer's growth or terminates the chain, because this ensures that the polymer chain is long. Chain length is critical: if the chains are too short, the polymer will be an oily wax-like substance rather than a solid plastic.

Calculating the PES

How do we calculate the PES? There are two popular methods, one based on rigorous *quantum mechanics* calculations and the other based on more approximate methods called *molecular mechanics*.

The QM approach. Solving the quantum mechanical Schrödinger equation or equivalent is one of the most direct methods of determining the PES. Approximate solutions to the Schrödinger equation are obtained at varying degrees of accu-

racy, with more accurate treatments generally requiring more computational effort. It is possible for the chemist to achieve experimental accuracy or better. The Schrödinger equation can be solved at varying degrees of accuracy, with more accurate treatments generally requiring more computational effort.

In principle, we can determine the entire PES for any system using QM methods; however, this is a computationally demanding process. Consequently, relatively small molecular systems are usually subject to this rigorous analysis.

Currently, the method of choice for QM simulations is *Kohn–Sham density functional theory*, because it provides a favorable balance between accuracy and speed. DFT calculations work for systems with thousands of atoms; however, molecular systems of approximately 100 atoms are the maximum for thoroughly studying the entire catalytic cycle's PES.

As an additional advantage, QM calculations produce a detailed electronic structure of the catalytic system. This can provide another avenue for rational catalyst design.

The MM approach. Molecular mechanics is another popular method for determining the PES of a molecular system. The MM approach is drastically different from the QM approach. Instead of blanketing the nuclei with a complicated electronic structure, the PES is determined from a set of simple, predetermined mathematical functions parameterized to fit experimental results. Conceptually, the molecular system is like a set of billiard balls connected by springs, with the springs representing the molecular bonds.

In this case, simplicity is a virtue. MM can effectively handle systems that are orders of magnitude larger than those QM can solve. Thus, it is possible to simulate whole proteins composed of tens of thousands of atoms.

MM's primary drawback is that bond breaking and forming processes are not accurately simulated. Unfortunately, the formation of new bonds as the monomer units join is at the core of the polymerization process.

Building a realistic computational model

Computational modeling of olefin polymerization catalysis requires a high-level QM treatment. The speedier lower-level MM approaches cannot accurately treat the bond breaking and forming processes that take place during the catalytic cycle. The down side is that QM requires tremendous computational resources.

Due to the expense of QM calculations, the detailed study of a catalytic cycle often involves a stripped down model of the chemical system. Figure 3 provides an example: Figure 3a depicts the real catalytic system while Figure 3b shows a likely model used for a QM-level calculation (the peripheral components of the catalyst and the solvent are removed). In some cases, such peripheral components act only as spectators, but in others, they can substantially influence the PES. Thus, QM models that neglect the surrounding molecular environment might lead to limited or even erroneous conclusions.

The combined QM/MM approach

One popular approach to simulate complex molecular systems at the quantum mechanical level is the combined quantum mechanics and molecular mechanics (QM/MM) method.³⁻⁵ In this hybrid method, part of the molecular potential, such as the catalyst's active site, is determined by a QM calculation while the remainder of the molecular potential is determined using a much faster MM calculation (see Figure 3c). The QM/MM method's promise is that it allows for simulations of bond breakage and formation at the active site, while still taking into account the role of the extended system in an efficient and computationally tractable manner.

The QM/MM method's key feature is that a QM calculation is performed on a truncated QM model of the active site (Figure 3b) with the large ligands removed and replaced by capping atoms. Then, a MM calculation is performed on the remainder of the system. The effects of the attached ligands form the entire system's PES where the QM and MM regions interact with one another through steric and electrostatic potentials.

One common simulation strategy for treating large and complex systems involves combining microscopic simulation techniques with mesoscopic or macroscopic ones. These multiresolution methods simultaneously span many orders of magnitude of length scales. In general, the hybrid QM/MM remains at the microscopic level so that the catalytic system is treated at the atomic level. What varies is that we move from a *fine-grain* Hamiltonian (the QM region) to a *course-grain* Hamiltonian (the MM region).

One of the first applications of the combined QM/MM method to studies of olefin polymerization involved the catalyst system Figure 3 depicts. The nickel-based catalyst was developed in the laboratory of Maurice Brookhart and first published in 1995.⁶ At the time, the system was

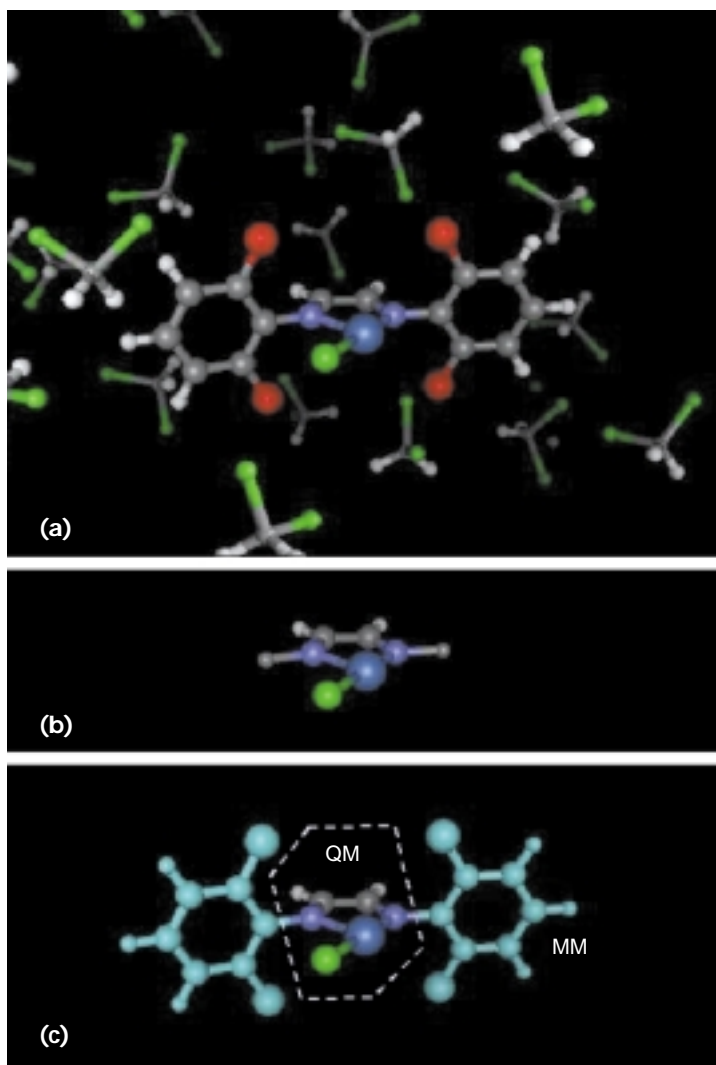


Figure 3. Real catalytic systems and their computational models: (a) a catalyst system with large flanking substituents, including the surrounding solvent molecules; (b) a common computational model performed at the QM level, with the peripheral groups truncated to reduce the computing effort required; and (c) a combined quantum mechanics and molecular mechanics model (within the dashed line), including the flanking substituents treated with less computationally demanding methods.

too large to treat wholly at the QM level. Unfortunately, the bulky substituents that flank either side of the active site (shown in blue, Figure 3c) are critical to the catalyst's performance. Without them, the catalyst is completely ineffective in polymerization.

In initially studying the system, we used the truncated model system shown in Figure 3b in a pure QM study. The flanking substituent groups were too large to treat at the QM level. In agreement with experimental results, the calculated PES revealed that no polymerization

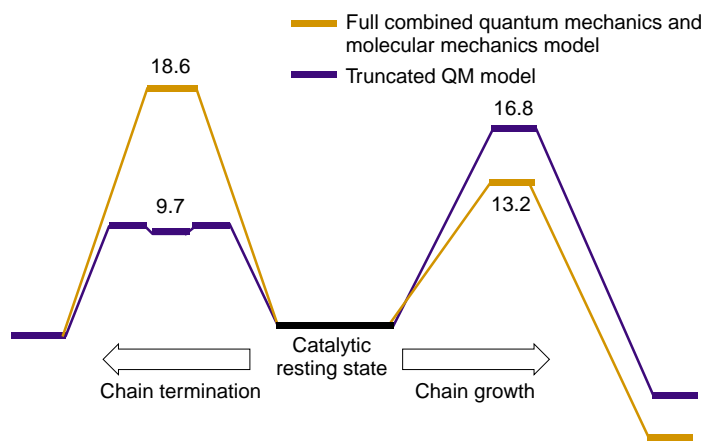


Figure 4. Calculated potential energy profile of the chain growth and termination processes of Maurice Brookhart's olefin polymerization catalyst. Calculations for the profile in blue used a truncated model system, neglecting the flanking substituents. Calculations for the profile in green used the combined quantum mechanics and molecular mechanics method, accounting for the flanking substituents. The effect of the substituents, both calculated and experimentally, is dramatic.

should occur with the catalyst. The barrier for the chain growth process was much larger than the chain termination's barrier. Figure 4 depicts the potential energy surface in blue.

Because it is not feasible to simulate the entire catalyst system at the QM level, the combined QM/MM method accounted for the influence of the flanking substituents on the PES. The change was dramatic (see the green potential energy surface in Figure 4).⁷ The bulky ligands doubled the barrier to chain termination, thereby making chain growth a more favorable process than termination—a minimum requirement for a polymerization catalyst. In addition to information about the PES's basic features, the combined QM/MM simulation provided detailed insight into how the catalyst operated at the atomic level. This paves the way for rational improvement of the system. In addition, the combined QM/MM study was also accurately able to estimate the barrier heights later shown to compare favorably with experimental values.^{7,8}

Adding the dynamic dimension

We can classify conventional quantum chemical calculations as static simulations. In these simulations, the PES is mapped out at the zero temperature limit; however, the finite temperature-free energy surface is directly related to properties derived from laboratory experimentation. For many

processes, the features of the finite temperature-free energy surface and the zero-Kelvin potential surface are nearly identical; thus, excluding finite temperature effects is a valid approximation. However, for other processes, the features of the two surfaces can deviate significantly.

One common approach to accessing finite temperature-free energies is through a molecular dynamics simulation. With molecular dynamics, the nuclei move on the zero-Kelvin potential energy surface according to Newton's classical equations (such as $F = ma$) to simulate the motion at the specified temperature. Unfortunately, it is not possible to solve these equations analytically; we must solve them iteratively in small time steps. For example, a relatively short 10 ps simulation typically requires 10,000 time steps. At each of these time steps, the force, F , on each nuclei is required. Performed at the QM level, this would require solving the Schrödinger equation for each time step, which is an exceptionally demanding task for all but the smallest systems.

In 1985, Roberto Car and Michele Parrinello^{9,10} developed a clever approach that allows molecular dynamics simulations performed at the QM level to be practical. The trick with the Car–Parrinello method is the electronic system or wave function that blankets the nuclei propagates synchronously with the nuclei so that they also follow Newton's equations of motion. This effectively eliminates the need to solve the Schrödinger equation at each time step. The Car–Parrinello method and other methods that use similar strategies are collectively termed *ab initio molecular dynamics* methods.

We have studied olefin polymerization catalysis using the AIMD approach. In addition to using the method to access finite temperature-free energies,¹¹ we found it a useful computational tool for determining time scales of processes and efficiently exploring complicated PES.

One brief example of how we used the AIMD method to determine the finite temperature behavior of a molecular interconversion process follows. During the polymerization process, the growth of the polymer chain occurs on the metal center of the catalyst. Because the metal center in these catalyst systems is electron deficient, it is often stabilized by an interaction with one of the hydrogen atoms in the growing chain. These so-called agostic interactions can occur between the metal and any of the hydrogen atoms along the growing chain. It is of interest to know which of the hydrogen atoms the metal atom prefers and whether there is any interconversion between structures.

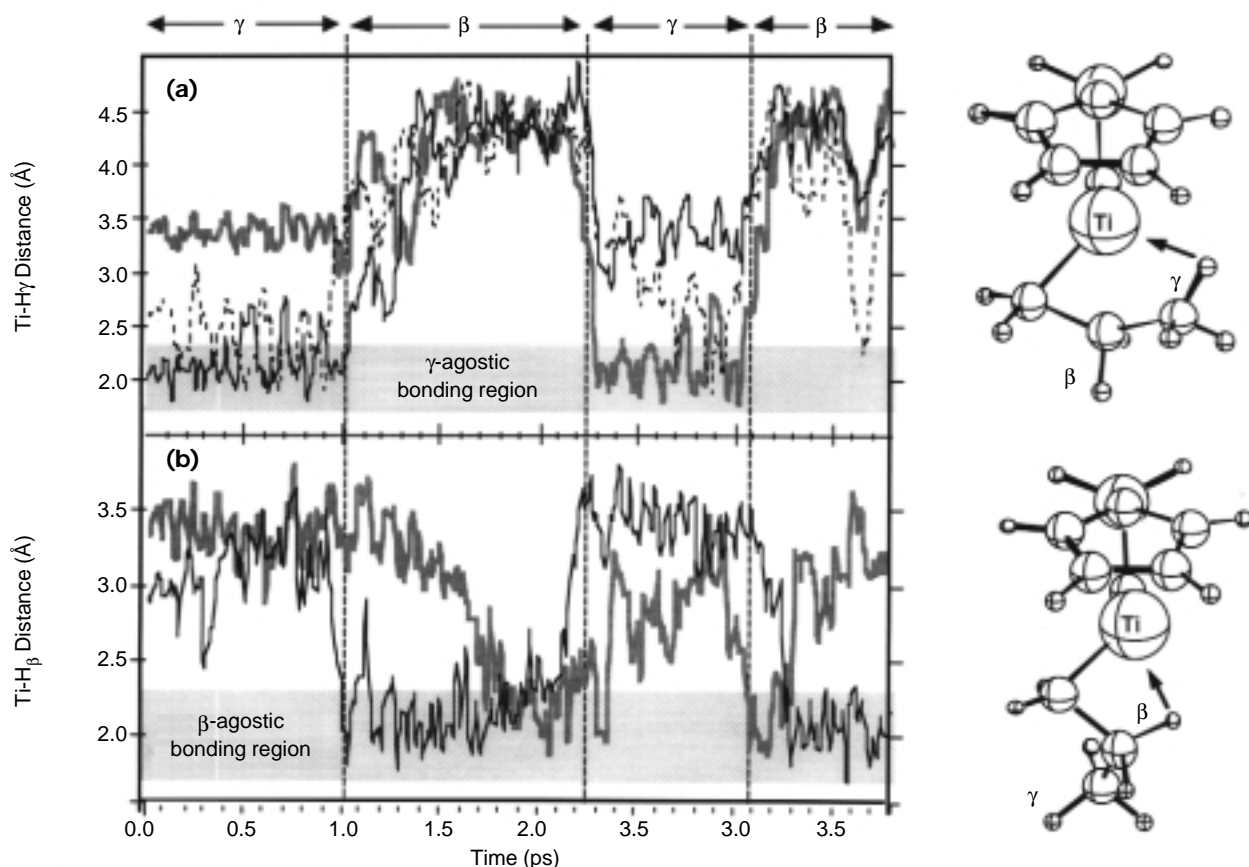


Figure 5. Selected Ti-H distances during the Car-Parrinello ab initio molecular dynamics simulation of a Ti-growing chain model. Shaded regions indicate the so-called agostic bonding between hydrogen and metal. Vertical lines separate where the complex can be characterized as beta- and gamma-agostic complexes. Shown on the right are two snapshot structures taken from the simulation characteristic of the gamma-agostic (top) and beta-agostic complexes (bottom).

We applied the AIMD method to examine this issue for a specific titanium-based olefin polymerization catalyst. The right-hand side of Figure 5 shows two preferred agostic interactions between hydrogen atoms of the growing polymer chain and the metal center. We can designate carbon atoms as α , β , γ , and so forth, depending on their proximity to the metal center along the growing chain's backbone. Two preferred conformations are ones in which a hydrogen atom on the γ -carbon interacts with the metal center and one in which a hydrogen atom on the β -carbon interacts. We have performed a Car-Parrinello AIMD simulation of these complexes at room temperature. Figure 5 shows various Ti-H distances monitored during the simulation. The Ti-H distances in the shaded regions indicate an agostic interaction. The simulation reveals that there is a rapid interconversion between the γ -agostic and β -agostic complexes.

Furthermore, when an γ -agostic interaction is lost, another γ -agostic bond immediately replaces it or the system immediately converts to β -agostic conformation. Thus, even at finite temperatures, the strong preference for the formation of agostic interactions stabilizes the process.

Chemical supercomputing on the cheap

There has always been a strong connection between computational chemistry and high-performance computing. Thus, a necessary yet often understated aspect of computational chemistry involves the cost-effective management of computing resources. This is particularly true for quantum chemists using computationally demanding methods. This fact has traditionally confined high-level calculations to large and expensive vector and parallel supercomputers.

To provide higher processing capability at a



Figure 6. Cobalt, a Beowulf-class supercomputer built from 94 commodity workstations.

lower cost, a recent trend is to construct a Beowulf supercomputer (www.beowulf.org), which is comprised of a cluster of lower-cost, commodity-type computers such as those with Intel's Pentium processors. Although a Beowulf supercomputer might not be appropriate for all applications, we found that it met our quantum chemistry needs exceptionally well and at a lower cost.

We built and optimized a Beowulf supercomputer, Cobalt, for quantum chemistry applications (see Figure 6). We chose the name because Cobalt, the 27th element in the periodic table, is an important transition metal used in many catalytic processes. Ninety-four Compaq/DEC Alpha personal workstations comprise Cobalt. Each node contains an Alpha 21164A processor running at 500 MHz with between 64 and 512 Mbytes of memory. We purchased this equipment between March 1998 and February 1999 for US \$220,000 (an average of \$2,340 per node). We also used off-the-shelf networking software and hardware. Each node communicates through a dedicated 96-port full duplex 100BaseTx Ethernet switch constructed from four 24-port switches. The cost of the networking hardware was only \$9,200. Thus, including software and miscellaneous expenses of \$4,420, the cost of the Cobalt cluster totaled \$233,620 or roughly \$2,500 per Gflop of peak performance.

With rapid advances in the commodity processor market and with high-speed gigabit networking technology becoming more mainstream, the Beowulf approach is accessible to research groups with modest budgets. It is also a

good long-term solution and investment, primarily because it can be easily and reasonably upgraded as new software and equipment is available. Any of the latest and greatest commodity-type computers can join the existing heterogeneous array. Therefore, no particularly large sum of money is required to enhance the cluster's power—any level of investment feasibly improves performance over time.

Traditional quantum chemical calculations on Cobalt

For the traditional quantum chemical calculations that map out the reactions at the zero-Kelvin limit, we use the Amsterdam Density Functional (ADF) quantum chemistry package (partially developed within our group). As in most traditional quantum chemistry packages, it uses atom-centered basis functions to construct the wave function and electron density.

For the system sizes that we typically calculate (about 100 atoms in the QM region), the computational bottleneck is the construction of the matrix of the Kohn–Sham operator (sometimes called the Fock matrix). In ADF, the 3D numerical integration of real space grid points completely determines the matrix. This differs from many other quantum chemistry packages that analytically evaluate most or all the necessary integrals.

In ADF, the full numerical integration allows straightforward parallelization. The integration grid points are simply distributed amongst the individual nodes. Using either the MPI or PVM message-passing libraries, parallelization occurs only for the computationally intensive parts of the program, namely the numerical integration. All relatively inexpensive parts of the calculations repeat on all participating nodes, so the nodes need to synchronize and communicate relatively infrequently. This somewhat atypical parallelization procedure greatly reduces network traffic, making the commodity networking hardware used in Cobalt more than adequate.

Figure 7 illustrates the parallel performance of QM calculations using ADF on the Cobalt cluster with the full geometry optimization of a 38-atom nitridoporphyrinatochromium complex. The single-node calculation required approximately 11.4 hours using 45 Mbytes of memory and approximately 100 Mbytes of disk space. Figure 7 shows the scaling of the calculation up to 16 nodes. Considering the complexity of the quantum chemistry code, we find the scaling very favorable.

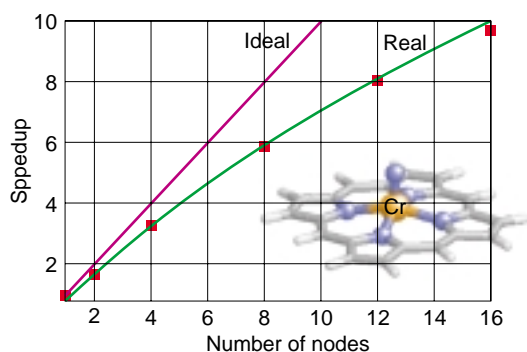


Figure 7. The parallel performance of the Amsterdam Density Functional quantum chemistry package compared to an ideal scaling, using the nitridoporphyrinatochromium molecule as a test case.

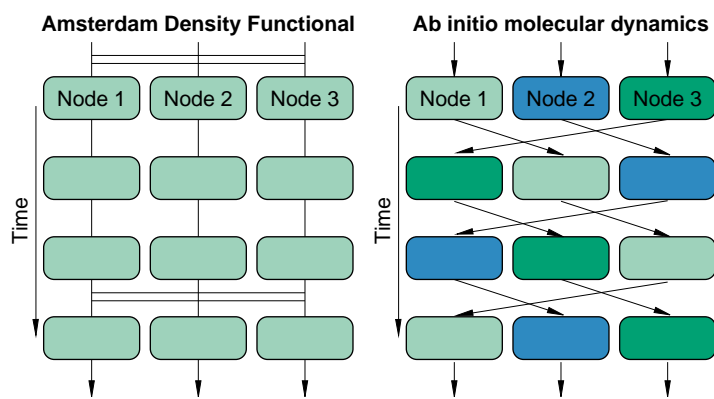


Figure 8. The internode communication during a parallel Amsterdam Density Functional simulation compared with an ab initio molecular dynamics simulation.

Ab initio molecular dynamics calculations on Cobalt

For the Car–Parrinello AIMD calculations, we used the CP-PAW program.¹² Although the Car–Parrinello approach is also based on Kohn–Sham DFT, it differs from many traditional quantum chemistry packages. It uses plane wave basis functions to represent the wave function and electron density as opposed to atom-centered basis functions. The result is that the necessary integrations required to construct the Kohn–Sham matrix are minute on a per function basis if it is done in a Fourier representation. On the other hand, orders of magnitude more basis functions are required compared to using atom-centered basis functions. Thus, 3D complex fast Fourier transforms (FFTs) computationally dominate the AIMD simulations.

In terms of parallelization, the AIMD simulations are the exact opposite of ADF and most other traditional quantum chemistry codes. The FFTs place a heavy demand on both internode bandwidth and roundtrip latency. For example, when running on N nodes, the parallel FFT algorithm needs to exchange all Fourier coefficients on each node N times during each molecular dynamics time step. Figure 8 compares the internode communication during an ADF and AIMD simulation.

The resulting heavy communications traffic stresses the commodity-type networking

used in the Cobalt cluster, and the AIMD calculations do not scale as well as the ADF simulations. Figure 9 shows the parallel performance of a medium-size molecular system of CH_3I and $[\text{Rh}(\text{CO})_2\text{I}_2]$. We found that a parallel simulation using 10 or more Cobalt nodes no longer runs efficiently, because the network becomes choked. At the same time, as higher-speed gigabit Ethernet technologies become more economical, the scaling of the AIMD simulations on a Beowulf-class computer should improve.

In another difference from traditional quantum chemical calculations, AIMD simulations have a much larger memory footprint and are often limited by memory requirements. Thus, in addition to distributing the computational effort, parallelization provides the additional advantage of distributing the memory requirements among the nodes. For example, a parallel AIMD job requiring 3 Gbytes of memory can run in parallel on Cobalt even though no node has more than 512 Mbytes

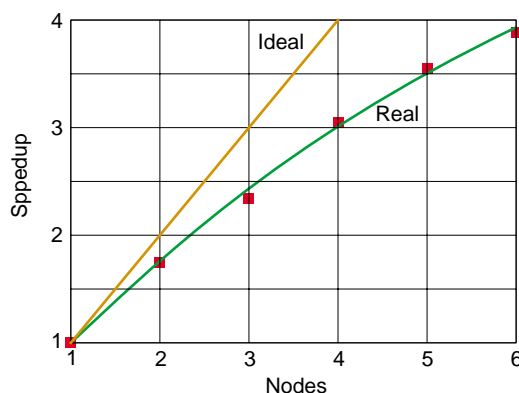


Figure 9. Parallel performance of an ab initio molecular dynamics simulation on Cobalt using commodity 100baseT networking compared to an ideal scaling.

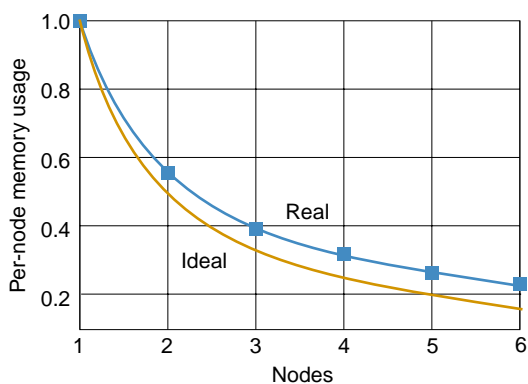



Figure 10. The scaling of the memory requirements with an ab initio molecular dynamics simulation on Cobalt.

of memory. The memory overhead of a typical AIMD simulation is very small. Figure 10 shows a close to ideal memory distribution for an AIMD simulation; the single node job requires 231 Mbytes of memory.

Modeling polymerization at the atomic level is a challenging yet important source of information that will contribute to breakthroughs in the development of new catalysts and new plastics. With recent developments in theoretical methods coupled with the rapid decrease in the cost of pure number crunching, computational chemistry is becoming a cost-effective research tool. In both academia and industry, opportunities abound for the refinement of existing and the development of new olefin polymerization catalysts.

We are currently developing techniques to incorporate the effects of the solvent that surrounds the catalyst systems during the polymerization process. We also hope to develop rapid screening techniques to sift out bad candidate catalysts before they are synthesized in the lab. The challenge here involves developing a reliable yet relatively easy-to-calculate metric to screen the catalysts.

In the future, we foresee realistic, atomic-level modeling of increasingly complex systems. As a result, more detailed insight into a broader range of chemical systems will be possible. 

Acknowledgments

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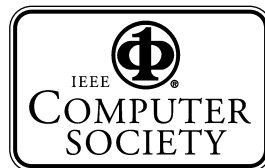
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