chapter

1 The Art of Problem Solving

Modern supercomputers can perform billions of calculations in a single second. With such computing power available, why do scientists need even faster computers to solve some problems?

Consider the question of how a steel beam supporting a bridge might fracture under extreme stress. To approach this problem, a new science called **molecular dynamics** is being used to model the motion of individual atoms in the metal. Modeling a rectangular slab of metal only 1000 atoms wide, 2000 atoms long, and 19 atoms thick requires over 50 hours for a supercomputer. In order to simulate the motion of 100 million atoms in a steel beam, 7.6 billion numbers must be stored in computer memory. Because an atom's movement is so rapid, scientists must calculate its velocity and location every 1 millionth of 1 billionth of a second. Each one of these steps in time takes 90 billion arithmetic calculations. Scientists have so far succeeded in modeling 600 million atoms at one time. But, a single speck of dust can contain more than a billion atoms, so only extremely small pieces of metal can currently be modeled. Modeling an entire steel beam as it fractures under stress is not within reach of today's supercomputers simply because they are too slow.

Real applications requiring high-speed computation are becoming increasingly important. From modeling the heart over long periods of time to predicting weather 24 hours in advance, real-world problems are indeed very complex. Understanding them will require not only faster computers, capable of performing trillions rather than billions of calculations per second, but also new problem-solving strategies.

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