Professor Joseph Traub is best known as a pioneer in the computational complexity of continuous problems. This involves understanding the least amount of resources—time, memory, communications—needed to solve a computing problem.

“My strategy is to start a new area of research or get into something fairly early. Then I can just walk along and pick up diamonds of knowledge and insight. I never have to strip mine for them,” he said.

It is probably as good a background as any for his investigations into the potential of quantum computing. It is a quest at the intersection of physics, mathematics and computer science.

Quantum computing stands conventional computing on its head. For example, bits are the basic unit of information in today’s computers. They can have one of two values, either zero or one, which microprocessor transistors represent as on or off.

Quantum computers are built around qubits, which have a property called superposition. This means they can be in many quantum states between zero and one, all at the same time. The more qubits a processor has, the more potential states it allows.

Qubits also have a property called entanglement. For reasons not yet understood, changing the quantum state in one of two entangled particles instantaneously changes it in the other. “That enables qubits to work together without wires,” Traub said.

Because quantum computers are not limited to on-off states, they can calculate many possible answers at once. This could make it possible to calculate very complex problems rapidly.

“What I’m trying to do is ask, ‘Where are the big wins?’ In particular, what kind of problems could a quantum computer solve that physicists and chemists are really interested in solving,” Traub said.

One of those problems is calculating the lowest energy state, or ground state energy, of a large number of particles. “This is a central problem in computational chemistry, and it would allow us to predict chemical reactions better,” Traub explained.

The problem, he explained, is that ground state energy calculations are difficult and soak up computer resources. A quantum computer’s ability to make multiple calculations simultaneously could give chemists the tool they need to predict particle interactions in large systems.

“We’re theoreticians, trying to understand the type of problems quantum computers might be able to solve. Physicists may never succeed in building one, but if they do, we want to be ready,” Traub concluded.

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