

MODELING MILLIONS OF ATOMS AND THEIR ELECTRONS: TIGHT-BINDING USING A SPECTRAL PROJECTION PURIFICATION METHOD

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EXECUTIVE SUMMARY

In this project, we demonstrated a new method for accurately computing properties of material systems containing up to 10 million atoms and their electrons. The method is based on a linear scaling version of tight binding, which is a semiempirical approach for computing, from a model, the energy of a collection of atoms for the interactions among the electrons and the nuclei. We computed the density matrix—a fundamental property of such a system—using a spectral projection purification method. The method scaled well on Blue Waters to millions of atoms over thousands of processors. As an example, we computed the electronic properties of an SiO₂ crystal, which we reported in the form of the density of states. The results show the feasibility of the approach as a general-purpose total-energy electronic structure computational tool for materials science.

RESEARCH CHALLENGE

Our interest is in testing more efficient methods for computing the electronic structure of systems with millions and tens of millions of atoms. Properties of material domains of this size are important in many different technologies, from microelectronics to medical science to energy technologies. Our interest is in the properties of dielectric materials of plasma generation, which are important in combustion, materials processing, and catalysis. Traditional electronic structure calculations for these kinds of materials have cubic scaling in N —the number of atoms in the system—making the calculations prohibitively computationally expensive for systems larger than 10⁴ atoms.

METHODS & CODES

We used the code we developed to compute the density matrix, a fundamental electronic structure quantity for a system of atoms and their electrons. Our computational method [1] combines the advantages of two existing linear scaling methods: the Kernel Polynomial Expansion (KPE) [2] and second-order spectral projection purification (SP2) [3]. The KPE method is computationally efficient and can be easily expressed in terms of sparse matrix–vector multiplications (SpMVs), but cannot satisfy one of the required constraints on its own. On the other hand, the SP2 method is highly accurate but can be prohibitively costly in terms of memory and communication when expressed in terms of sparse matrix–matrix multiplications (SpGEMM). When

expressed in terms of SpMVs, the SP2 method scales exponentially with the number of iterations required to converge. An advantage of SP2, however, is that near the correct solution P , the method converges quadratically [3]. Thus, we have constructed a hybrid method that takes the inexpensive KPE solution and purifies P_{kpe} with a few SP2 iterations that are more expensive.

RESULTS & IMPACT

Our recent work has shown the feasibility of this method for computing properties of million-atom systems [1]. We will apply the method and have impact in the area of surface and dielectric properties for combustion, catalysis, and materials processing. The method can also have impact in other areas of physics and materials science. With the scaling observed during the outcome of the Blue Waters work, we have demonstrated that this method is fast, accurate, and efficient in 10-million-atom systems and beyond, which will increase its impact significantly.

WHY BLUE WATERS

Access to the Blue Waters system made this work possible by permitting our studies on a single platform that offered both large parallelism and resources for memory-intensive computations. Depending upon the tuning of the method, it is possible to carry out the entire computation on a single node in a very memory-intensive approach or, by distributing the computation over many processors, it is possible to perform the algorithm in a massively parallel way. The Blue Waters system allowed us to study the approach and plan for future studies with more optimized tuning.

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50-nm-long wire with a 3-nm diameter requires around 1 teraflop for a single energy point where more than 1,000 energy points are needed. And this calculation must be repeated perhaps a hundred times for a full current–voltage sweep. The treatment of a realistic device would require an atomistic resolution of a device with a cross-section of more than (20 × 20) nm², which includes the core semiconductor and the surrounding gate material. Such devices of larger sizes are especially an issue due to the $O(n^2)$ scaling of matrix operation time-to-solution and $O(n^2)$ scaling of memory. Blue Waters was used for running such simulations on up to 16,384 cores per simulation. In many cases, the work could not be accomplished in a reasonable amount of time without Blue Waters, and for the larger simulations the work could not be accomplished on other available systems. Blue Waters' staff provide exemplary support and user outreach to guide system usage, help with issues as they arise, and assist with code performance and scaling.

PUBLICATIONS & DATA SETS

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