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ELECTRONIC STRUCTURE OF MICROSCALE DIELECTRIC BARRIER DISCHARGES

Allocation: Illinois/350 Knh
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EXECUTIVE SUMMARY

The research team conducted high-throughput simulations to predict rates of electron emission from dielectric surfaces under AC voltage. By spanning a large range of dielectric barrier discharge (DBD) operating conditions, the team produced a data set that is the first of its kind for DBD plasma generators. The work relies on a method the researchers developed previously for the accurate simulation of material systems containing up to ten million atoms and their electrons. The study also tested the feasibility of numerical integrators for slow, nonperturbative electron dynamics and showed that adaptive numerical integrators perform better than expected. This observation demonstrates that it is possible to leverage numerical engineering methods to optimize or design dynamic electron systems such as DBD plasma generators.

RESEARCH CHALLENGE

The research aims to extend the length and timescales of atomistic, quantum–mechanical materials simulation, particularly of systems containing millions and tens of millions of atoms, under slow, nonperturbative, realistic AC voltages. Materials and phenomena in these temporal and spatial domains are important in many different technologies, from microelectronics to medical science to energy technologies. Traditional electronic structure calculations at this scale are constrained by memory and communication overheads, as they were designed to minimize the number of FLOPs. The research team's approach prioritizes memory and communication constraints as more limiting, and that is the reason they can simulate ten-million-atom systems on 100 nodes within a few minutes. The team has also taken a similar approach toward extending simulated timescales of electronic systems, with promising results. As a testbed application, the researchers have chosen to investigate dielectric surfaces in dielectric barrier discharge plasma generators, which are important in combustion, materials processing, and catalysis.

METHODS & CODES

The simulations use density-functional-based tight-binding, which is a semiempirical electronic structure method. The main computational workflow is to read the atomic coordinates, construct the Hamiltonian, and compute the required eigenspace that denotes the ground state of electrons.

Extending system size. In order to simulate million-atom systems, the team implemented its algorithm [1] using the PETSc distributed matrix library [2]. They used the code they developed to compute the density matrix, which is a fundamental electronic structure quantity for a system of atoms and their electrons. This computational method [1] combines the advantages of two existing linear scaling methods—the kernel polynomial expansion (KPE) [3] and second-order spectral projection purification (SP2) [4] methods. 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. 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 the method converges quadratically near the correct solution P [4]. Thus, the researchers have constructed a hybrid method that takes the inexpensive KPE solution and purifies P_{kpe} with a few SP2 iterations that are more expensive.

Extending timescales. The research team tested implicit–explicit time-steppers based on [5] within PETSc and found them to be appropriate for simulating 400-site electronic systems driven by slow, nonperturbative AC fields. This is significant because quantum–mechanical forward-time simulations are usually done using specialized explicit integrators [6–8]. Numerically, the team found that appropriately tuned implicit–explicit time-steppers conserve the invariants of electronic motion given in [9]. However, these temporal simulations currently scale quadratically with the number of sites, and future algorithmic work will be necessary to improve performance.

High-throughput simulations of small systems. The researchers built upon their electronic structure code, producing a data set for physical systems corresponding to pressures ranging from 10 Pa to 10 GPa and for electric fields between 10 V/m to 1 MV/m. The main computational bottleneck here was the size of data generated as well as constraints on wall-time. The constraint on wall-time was not prohibitive, but it limited the number of physical AC cycles that were averaged to produce the data set.

RESULTS & IMPACT

The team's recent work expands the scope of atomistic electronic structure simulations, extending the boundaries of the realm of feasible simulations. This allows researchers to simulate larger, more heterogeneous systems that are essential to understanding, designing, and optimizing complex devices and phenomena, directly affecting research on surface and dielectric properties for combustion, catalysis, and materials processing.

WHY BLUE WATERS

Access to the Blue Waters system made this work possible by permitting studies on a single platform that offered both large parallelism and resources for memory-intensive computations. Depending on the tuning of the method, it is possible to either carry out the entire computation on a single node, in a very memory-intensive approach, or, by distributing the computation over many processors, to perform the algorithm in a massively parallel way. The Blue Waters system allowed the team to study these approaches and to plan for future studies with more optimized tuning. The scale of Blue Waters also allowed them to extend the boundaries of possible electronic systems and phenomena that can be simulated in the future. In addition, they benefitted from the smooth, transparent, and dependable access to various system modules, as well as helpful and timely responses from Blue Waters staff.

PUBLICATIONS & DATA SETS

P. Ghale and H. T. Johnson, "Dielectric surface boundaries for plasma generators—parameterization of rates of electron emission from quartz under AC voltage," in preparation, 2020.

P. Ghale and H. T. Johnson, "Benchmarking implicit-explicit integrators for direct evolution of many-electron systems under slow, non-perturbative dynamical loading," in preparation, 2020.