Scalable Atomistic Simulation Algorithms for Materials Research

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Abstract

A suite of scalable atomistic simulation programs has been developed for materials research based on space-time multiresolution algorithms. Design and analysis of parallel algorithms are presented for molecular dynamics (MD) simulations and quantum-mechanical (QM) calculations based on the density functional theory. Performance tests have been carried out on 1,088-processor Cray T3E and 1,280-processor IBM SP3 computers. The linear-scaling algorithms have enabled 6.44-billion-atom MD and 111,000-atom QM calculations on 1,024 SP3 processors with parallel efficiency well over 90%. The production-quality programs also feature wavelet-based computational-space decomposition for adaptive load balancing, spacefilling-curve-based adaptive data compression with user-defined error bound for scalable I/O, and octree-based fast visibility culling for immersive and interactive visualization of massive simulation data.

Keywords: Parallel computing, molecular dynamics, variable-charge molecular dynamics, quantum mechanics, density functional theory, load balancing, data compression

1 Introduction

Modern design of high-performance materials and devices focuses on controlling structures at diverse length scales from atomic to macroscopic [28]. Rich variety of atomistic simulation methods ranging from empirical molecular-

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dynamics (MD) simulations to *ab initio* quantum-mechanical (QM) calculations are expected to play an important role in scaling down engineering concepts to nanometer scales. Recent advances in computational methodologies and massively parallel computers have made it possible to carry out 10-100 million atom simulations of real materials and devices typically on 10-100 processors [1, 10, 38].

This paper describes our efforts to enable very large-scale atomistic simulations involving multibillion atoms by designing scalable and portable simulation algorithms [16]. In the next section, we describe linear-scaling parallel algorithms for MD and QM calculations. Section 3 discusses software tools to support billion-atom simulations. Results of benchmark tests are given in Sec. 4, and Sec. 5 contains conclusions.

2 Parallel atomistic simulation algorithms

We have developed a suite of scalable MD and QM algorithms for materials simulations. The linear-scaling algorithms encompass a wide spectrum of physical reality: i) classical MD based on a many-body interatomic potential model; ii) environment-dependent, variable-charge MD; and iii) self-consistent QM calculation based on the density functional theory (DFT).

2.1 Multiresolution molecular dynamics algorithm

In the MD approach, one obtains the phase-space trajectories of the system (positions and velocities of all atoms at all time) [31]. Atomic force laws for describing how atoms interact with each other is mathematically encoded in the interatomic potential energy, $E_{\mathrm{MD}}(\mathbf{r}^N)$, which is a function of the positions of all N atoms, $\mathbf{r}^N = \{\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N\}$, in the system. In our many-body interatomic potential scheme, $E_{\mathrm{MD}}(\mathbf{r}^N)$ is expressed as an analytic function that depends on relative positions of atomic pairs and triples [38]. Time evolution of $\mathbf{r}^N$ is governed by a set of coupled ordinary differential equations. For interatomic potentials with finite ranges, the computational cost can be made $O(N)$ using a linked-cell-list approach [31]. Our ***multiresolution molecular dynamics (MRMD)*** algorithm [25] also uses an approach called the multiple time-scale (MTS) method [21, 23, 37], which uses different force-update schedules for different force components to reduce the number of force evaluations.

For parallelization of MD simulations, we use spatial decomposition [25, 31]. The total volume of the system is divided into P subsystems of equal volume, and each subsystem is assigned to a processor in an array of P processors. To calculate the force on an atom in a subsystem, the coordinates of the atoms in the boundaries of neighbor subsystems are cached from the corresponding processors. After updating the atomic positions due to a time-stepping procedure, some atoms may have moved out of its subsystem. These atoms are migrated to the proper neighbor processors. With the spatial decomposition, the computation scales as N/P while communication scales in proportion to $(N/P)^{2/3}$ for an N-atom system.

2.2 Variable-charge molecular dynamics

Physical realism of MD simulations is greatly enhanced by incorporating variable atomic charges that dynamically adapt to the local environment [4, 35]. However, the increased realism of this ***variable-charge molecular dynamics (VCMD)*** is accompanied by increased computational complexity, $O(N^3)$, for solving a linear system to determine atomic charges at every MD step. We have reduced this complexity to $O(N)$ [20] by combining the fast multipole method (FMM) [12, 25] and an iterative minimization approach. In the FMM, the space is recursively divided into subsystems to form an octree data structure and the electrostatic field is computed recursively on the octree with $O(N)$ operations. To further accelerate the convergence, we have developed a multilevel preconditioned conjugate-gradient (MPCG) method [20] by splitting the Coulomb-interaction matrix into short- and long-range components and using the sparse short-range matrix as a preconditioner.

Tree-based algorithms such as the FMM have been used extensively to perform massively parallel computer simulations of gravitational systems in astrophysics [39]. The FMM has also been used in conjunction with the MTS in parallel MD simulations of materials [25] and biomolecular systems [15, 32]. Although these space-time multiresolution algorithms deal with $O(N^2)$ problems, their basic algorithmic structures can be reused for the $O(N^3)$ VCMD. For example, the computational cost of our VCMD code is amortized by reusing a doubly nested loop with associated neighbor-list construction for both the MTS method for time-stepping and multilevel preconditioning for determining charges [20].

2.3 Linear-scaling quantum-mechanical calculation based on the density functional theory

Empirical interatomic potentials used in MD simulations fail to describe chemical processes. Instead, interatomic interaction in reactive regions needs to be calculated by a QM method that can describe breaking and formation of bonds. An atom consists of a nucleus and surrounding electrons, and quantum mechanics explicitly treats the electronic degrees-of-freedom. The density functional theory (DFT) reduces the exponentially complex quantum problem to a self-consistent matrix eigenvalue problem,* which can be solved with $O(M^3)$ operations (M is the number of independent wave functions and is on the order of N) [13, 18, 27]. The DFT can be formulated as a minimization of the energy, $E_{QM}(\mathbf{r}^N, \psi^M)$, with respect to electron wave functions, $\psi^M(\mathbf{r}) = \{\psi_1(\mathbf{r}), \psi_2(\mathbf{r}), ..., \psi_M(\mathbf{r})\}$, subject to orthonormalization constraints.

Efficient parallel implementation of DFT is possible with real-space approaches based on higher-order finite differencing [6] and multigrid acceleration [3, 9]. We include electron-ion interactions using norm-conserving pseudopotentials [36] and the exchange-correlation energy in a generalized gradient approximation [29]. For larger systems (M > 1,000), however, the $O(M^3)$ orthonormalization becomes the bottleneck.

For scalable DFT calculations, linear-scaling algorithms are essential [11]. We have implemented an $O(M)$ algorithm [34] based on unconstrained minimization of a modified energy functional and a localized-basis approximation [19]. In the parallel ***linear-scaling density functional theory (LSDFT)*** algorithm, the computation time scales as $O(M/P)$ on P processors, whereas the communication scales as $O((M/P)^{2/3})$. This is in contrast to the $O(M(M/P)^{2/3})$ communication in the conventional parallel real-space DFT algorithm. Global communication for calculating overlap integrals of the wave functions (which scales as $M^2\log P$ in the conventional DFT algorithm) is unnecessary in the linear-scaling algorithm.

3 Software tools

Practical simulations involving multibillion atoms are associated with a number of computational challenges, which have been addressed by a number of software tools.

3.1 Wavelet-based adaptive computational-space decomposition for load balancing

Many MD simulations are characterized by irregular atomic distribution and associated load imbalance. We have developed a computational-space-decomposition approach to load balancing [22, 24]. This scheme partitions the system in a computational space, which is related to the physical space by a curvilinear coordinate transformation. (The computational space shrinks where the workload density is high and expands where the density is low, so that the workload is uniformly distributed.) The optimal coordinate system is determined to minimize the load-imbalance and communication costs. We have found that wavelet representation leads to compact representation of curved partition boundaries, and accordingly to fast convergence of the minimization procedure [22].

3.2 Spacefilling-curve-based adaptive data compression for scalable I/O

A 1.5-billion-atom MD simulation we are currently performing produces 150 GB of data per frame (or per minute), including atomic species, positions, velocities, and stresses. For scalable input/output (I/O) of such large datasets, we have designed a data compression algorithm [26]. It uses octree indexing and sorts atoms accordingly on the resulting spacefilling curve. By storing differences between successive atomic coordinates, the I/O requirement for the same error tolerance level reduces from $O(N\log N)$ to $O(N)$. An adaptive, variable-length encoding scheme is used to make the scheme tolerant to outliers and optimized dynamically. An order-of-magnitude improvement in the I/O performance was achieved [26] for actual MD data with user-controlled error bound [40].

Another important issue in data management is the analysis of simulation results.† For atomistic simulations of materials, a challenge is to extract topological defects such as dislocations from massive data with large thermal noises. Graph data structures have played an important role in analyzing atomistic data [2, 7, 14], where vertices and edges represent atoms and bonds, respectively. Recently, we have used a shortest-path ring analysis to study intermediate-range orders in amorphous materials [8] and an edge-based indexing to detect grain boundaries in semiconductors nanocrystals [17].

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*Walter Kohn received a 1998 Nobel chemistry prize for the development of the DFT.

†For an extensive list of analysis tools for MD simulations, see http://www.ks.uiuc.edu/Research/MMTools.

3.3 Octree-based fast visibility culling for immersive and interactive visualization

Interactive exploration of large-scale atomistic simulations is important for identifying and tracking atomic features that are responsible for macroscopic phenomena, and an immersive and interactive virtual environment is an ideal platform for such explorative visualization, see Fig. 1.

We have developed a scalable visualization system to allow the viewer to walk through multimillion atoms [33]. The system uses fast visibility culling based on the octree data structure to reduce the number of atoms sent to the graphics pipeline. Multiresolution rendering is used to further speed up the rendering process. The resulting system renders a million-atom system at nearly interactive frame rates on a dual processor SGI Onyx2 with an InfiniteReality2 graphics pipeline. We are currently exploring the use of parallel preprocessing to achieve billion-atom walkthrough.

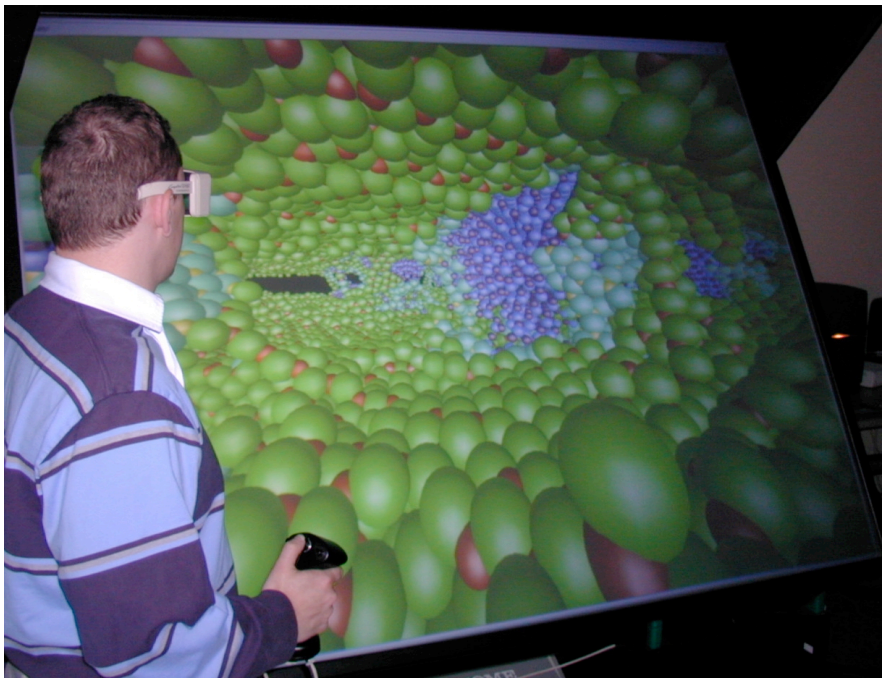

Figure 1: A researcher investigating a fracture in a 1.5-billion-atom model of a ceramic fiber composite material rendered in an ImmersaDesk virtual environment at our Concurrent Computing Laboratory for Materials Simulations.

4 Performance tests

Benchmark tests of the three parallel algorithms MRMD, VCMD, and LSDFT have been performed on the Cray T3E and the IBM SP3 computers at the U.S. Naval Oceanographic Office (NAVO) Major Shared Resource Center. All the three programs are written using MPI (Message Passing Interface) for message passing. The T3E at NAVO at the time of the benchmark tests consisted of 1,088 Digital Alpha processors with clock speed 450 MHz and 256 GB memory. The IBM SP3 at NAVO is configured with 375 MHz Power3 CPUs and has 334 nodes with 4 CPUs and 4 GB of memory per node.

Figure 2 shows the execution time of the MRMD algorithm for silica material as a function of the number of processors, P. In this algorithm, the interatomic potential energy is split into the long-range and short-range contributions, where the long-range contribution is computed after 10 steps. We scale the system size linearly with the number of processors, so that the number of atoms, $N = 648{,}000\,P$. On the T3E, execution time increases only slightly as a function of P, and this signifies an excellent parallel efficiency. On 1,024 processors, the parallel efficiency is as high as 97%. The computational time on the SP3 is significantly less than that on the T3E, but with increased communication time.

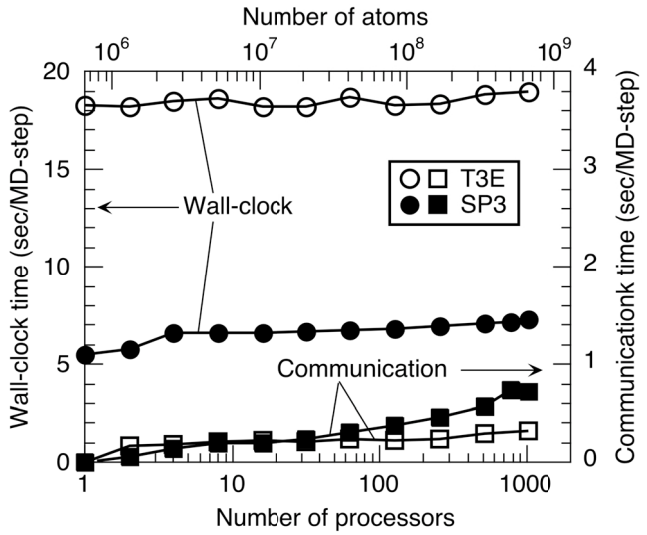

Figure 2: Wall-clock (circles) and communication (squares) times per time step of the MD algorithm with scaled workloads 648,000 P atom silica systems on P processors (P = 1, ..., 1,024) of Cray T3E (open symbols) and IBM SP3 (solid symbols).

Figure 3 shows the performance of the VCMD algorithm with scaled workloads 20,160 P-atom alumina systems on P processors (P = 1, ..., 1,024). Multipoles up to l_p = 6 are taken and the largest number of leaf octree cells is 8^6 (P = 1,024) in the FMM. The wall-clock time increases only slightly as a function of P, and the memory-bound parallel efficiency is 0.96 on 1,024 processors on the T3E.

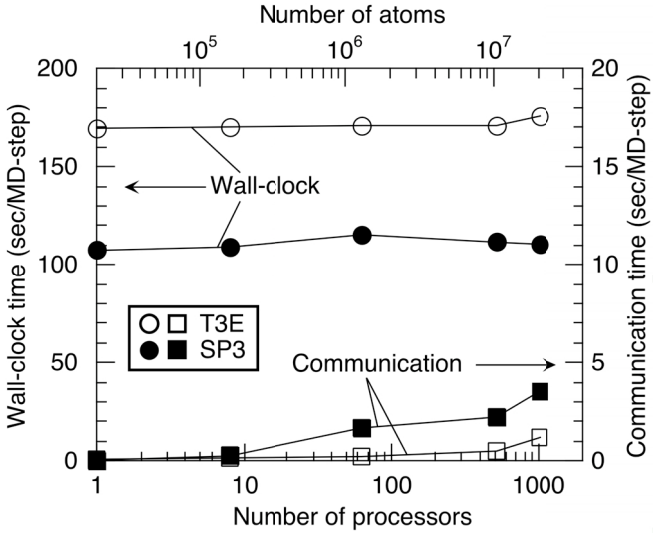

Figure 3: Wall-clock (circles) and communication (squares) times for the VCMD algorithm with scaled workloads 20,160 P atom alumina systems on P processors (P = 1, ..., 1,024) of Cray T3E (open symbols) and IBM SP3 (solid symbols).

In the LSDFT calculations for gallium arsenide material, the localization region for the wave functions is defined as a spherical space with radius 4.4 Å. Figure 4 shows the wall-clock and communication times per CG iteration on 1,024 T3E and SP3 processors. The wall-clock time scales linearly with N above $N \sim$ 10,000 (the number of wave functions, $M = 2N$). For the largest system (N = 110,592), the parallel efficiency is estimated to be 93%. The interprocessor communication scales as $O(N^{0.6})$ for $N >$ 10,000.

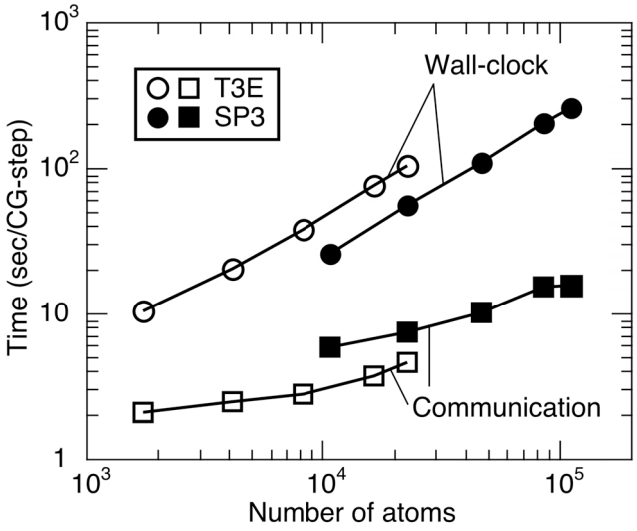

Figure 4: Wall-clock (circles) and communication (squares) times per CG step as a function of the number of atoms for the parallel LSDFT algorithm on Cray T3E and IBM SP3 computers. The system is gallium arsenide crystal in the zinc-blende structure. The number of processors is 1,024.

Major design parameters for MD simulations of materials include the number of atoms in the simulated system and the methodologies to compute interatomic forces (classically in MRMD, semiempirically in VCMD, or quantum-mechanically [5] in LSDFT). Figure 5 shows a design-space diagram for classical and quantum-mechanical MD simulations on 1,024 T3E and SP3 processors. (For the LSDFT, one MD step involves 3 self-consistent DFT iterations each consisting of 20 CG steps.) The figure demonstrates linear scaling for all the three algorithms, with prefactors spanning seven-orders-of-magnitude. The largest benchmark tests in this study include 6.44-billion-atom MRMD and 111,000-atom LSDFT calculations on 1,024 SP3 processors.

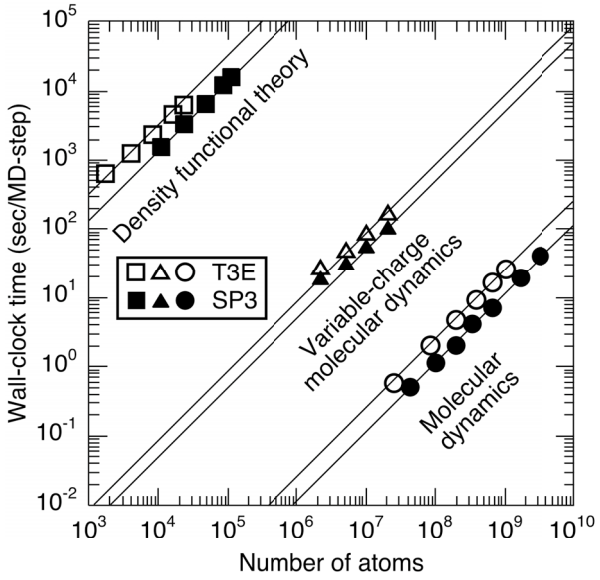

Figure 5: Design-space diagram for MD and QM simulations on 1,024 Cray T3E processors (open symbols) and on 1,024 IBM SP3 processors (solid symbols). The figure shows wall-clock time per MD step as a function of the number of atoms for three linear-scaling algorithms: Classical MD (MRMD, circles); environment-dependant variable-charge MD (VCMD, triangles); and, quantum-mechanical MD based on the DFT (LSDFT, squares). Lines show $O(N)$ scaling.

5 Conclusions

Modern MD simulations of materials started in 1964 when Aneesur Rahman simulated 864 argon atoms on a CDC 3600 computer [30]. Assuming a simple exponential growth, the number of atoms that can be simulated in classical MD simulations has doubled every 19 months to reach 6.44 billion atoms in this study. Similarly, the number of atoms in DFT-based *ab initio* MD simulations (started by Roberto Car and Michelle Parrinello in 1985 for 8 Si atoms [5]) has doubled every 12 months to 111,000 atoms in this study. Petaflop computers anticipated to be built in the next ten years will maintain the growth rates in these MD Moore's Laws, and we will be able to perform 10^{12}-atom classical and 10^{7}-atom quantum MD simulations on such computers. Multiresolution approaches used in our algorithms, combined with cache-conscious techniques, will be essential to achieve scalability on petaflop architectures.

Atomistic simulations have now reached a scale such that they must be performed in a metacomputing environment of geographically-distributed multiple supercomputers. Such efforts are underway on NASA's Information Power Grid (www.ipg.nasa.gov).

Acknowledgements

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References

[1] F. F. Abraham. Portrait of a crack: Rapid fracture mechanics using parallel molecular dynamics. *IEEE Computational Science & Engineering*, 4(2):66-77 (1997).

[2] M. J. Alava, P. M. Duxbury, C. F. Moukarzel, and H. Rieger. Exact combinatorial algorithms: Ground states of disordered systems. In *Phase Transitions and Critical Phenomena, Vol. 18*, eds. J. Lebowitz and C. Domb. Academic Press, London, 2000.

[3] T. L. Beck. Real-space mesh techniques in density-functional theory. *Reviews of Modern Physics*, 72:1041-1080 (2000).

[4] T. J. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, S. Ogata, and S. Rodgers. Dynamics of oxidation of aluminum nanoclusters using variable charge molecular-dynamics simulations on parallel computers. *Physical Review Letters*, 82:4866-4869 (1999).

[5] R. Car and M. Parrinello. Unified approach for molecular dynamics and density functional theory. *Physical Review Letters*, 55:2471-2474 (1985).

[6] J. R. Chelikowsky, Y. Saad, S. Ögüt, I. Vasiliev, and A. Stathopoulos. Electronic structure methods for predicting the properties of materials: Grids in space. *Phyica Status Solidi (b)*, 217:173-195 (2000).

[7] D. J. Cook, L. B. Holder, G. Galal, and R. Maglothin. Approaches to parallel graph-based knowledge discovery. *Journal of Parallel and Distributed Computing*, 61:427-446 (2001).

[8] I. Ebbsjö, R. K. Kalia, A. Nakano, J. P. Rino, and P. Vashishta. Topology of amorphous gallium arsenide on intermediate length scales: A molecular dynamics study. *Journal of Applied Physics*, 87:7708-7711 (2000).

[9] J.-L. Fattebert and J. Bernholc. Towards grid-based $O(N)$ density-functional theory methods: Optimized nonorthogonal orbitals and multigrid acceleration. *Physical Review B*, 62:1713-1722 (2000).

[10] T. C. Germann and P. S. Lomdahl. Recent advances in large-scale atomistic materials simulations. *Computing in Science and Engineering*, 1(2):10-11 (1999).

[11] S. Goedecker. Linear scaling electronic structure methods. *Reviews of Modern Physics*, 71:1085-1123 (1999).

[12] L. Greengard and V. Rokhlin. A fast algorithm for particle simulations. *Journal of Computational Physics*, 73:325-348 (1987).

[13] P. Hohenberg and W. Kohn. Inhomogeneous electron gas. *Physical Review*, 136:B864-B871 (1964).

[14] D. J. Jacobs and B. Henderson. An algorithm for two-dimensional rigidity percolation: The pebble game. *Journal of Computational Physics*, 137:346-365 (1997).

[15] L. Kalé, R. Skeel, M. Bhandarkar, R. Brunner, A. Gursoy, N. Krawetz, J. Phillips, A. Shinozaki, K. Varadarajan, and K. Schulten. NAMD2: Greater scalability for parallel molecular dynamics. *Journal of Computational Physics*, 151:283-312 (1999).

[16] R. K. Kalia, T. J. Campbell, A. Chatterjee, A. Nakano, P. Vashishta, and S. Ogata. Multiresolution algorithms for massively parallel molecular dynamics simulations of nanostructured materials. *Computer Physics Communications*, 128:245-259 (2000).

[17] S. Kodiyalam, R. K. Kalia, H. Kikuchi, A. Nakano, F. Shimojo, and P. Vashishta. Grain boundaries in gallium arsenide nanocrystals under pressure: A parallel molecular-dynamics study. *Physical Review Letters*, 86:55-58 (2001).

[18] W. Kohn and P. Vashishta. General density functional theory. In *Inhomogeneous Electron Gas*, eds. N. H. March and S. Lundqvist, pages 79-184. Plenum, New York, 1983.

[19] F. Mauri and G. Galli. Electronic-structure calculations and molecular-dynamics simulations with linear system-size scaling. *Physical Review B*, 50:4316-4326 (1994).

[20] A. Nakano. Parallel multilevel preconditioned conjugate-gradient approach to variable-charge molecular dynamics. *Computer Physics Communications*, 104:59-69 (1997).

[21] A. Nakano. Fuzzy clustering approach to hierarchical molecular dynamics simulation of multiscale materials phenomena. *Computer Physics Communications*, 105:139-150 (1997).

[22] A. Nakano. Multiresolution load balancing in curved space: The wavelet representation. *Concurrency: Practice and Experience*, 11:343-353 (1999).

[23] A. Nakano. A rigid-body based multiple time-scale molecular dynamics simulation of nanophase materials. *The International Journal of High Performance Computing Applications*, 13:154-162 (1999).

[24] A. Nakano and T. J. Campbell. An adaptive curvilinear-coordinate approach to dynamic load balancing of parallel multi-resolution molecular dynamics, *Parallel Computing*, 23:1461-1478 (1997).

[25] A. Nakano, R. K. Kalia, and P. Vashishta. Multiresolution molecular dynamics algorithm for realistic materials modeling on parallel computers. *Computer Physics Communications*, 83:197-214 (1994).

[26] A. Omeltchenko, T. J. Campbell, R. K. Kalia, X. Liu, A. Nakano, and P. Vashishta. Scalable I/O of large-scale molecular-dynamics simulations: A data-compression algorithm. *Computer Physics Communications*, 131:78-85 (2000).

[27] M. C. Payne, M. P. Teter, D. C. Allan, T. A. Arias, and J. D. Joannopoulos. Iterative minimization techniques for *ab initio* total energy calculations: molecular dynamics and conjugate gradients. *Reviews of Modern Phys*ics, 64:1045-1097 (1992).

[28] A. Pechenik, R. K. Kalia, and P. Vashishta. *Computer-Aided Design of High-Temperature Materials*. Oxford Univ. Press, Oxford, 1999.

[29] J. P. Perdew, K. Burke, and M. Ernzerhof. Generalized gradient approximation made simple. *Physical Review Letters*, 77:3865-3868 (1996).

[30] A. Rahman. Correlations in the motion of atoms in liquid argon. *Physical Review*, 136(2A):A405-A411 (1964).

[31] D. C. Rapaport. *The Art of Molecular Dynamics Simulation*. Cambridge Univ. Press, Cambridge, 1995.

[32] T. Schlick, R. D. Skeel, A. T. Brunger, L. V. Kalé, J. A. Board, J. Hermans, and K. Schulten. Algorithmic challenges in computational molecular biophysics. *Journal of Computational Physics*, 151:9-48 (1999).

[33] A. Sharma, P. Miller, X. Liu, A. Nakano, R. K. Kalia, P. Vashishta, T. J. Campbell, and A. Haas. Million atom walkthrough: Octree-based fast visibility culling and multiresolution rendering for scalable atomistic visualization. Computer Science Technical Report, Louisiana State University, 2001. [A shorter version has appeared in: A. Nakano, R. K. Kalia, and P. Vashishta. Scalable molecular-dynamics, visualization, and data-management algorithms for materials simulations. *Computing in Science & Engineering*, 1(5):39-47 (1999).]

[34] F. Shimojo, T. J. Campbell, R. K. Kalia, A. Nakano, P. Vashishta, S. Ogata, and K. Tsuruta. A scalable molecular-dynamics-algorithm suite for materials simulations: Design-space diagram on 1,024 Cray T3E processors. *Future Generation Computer Systems*, 17:279-291 (2000).

[35] F. H. Streitz and J. W. Mintmire. Electrostatic potentials for metal-oxide surfaces and interfaces. *Physical Review B*, 50:11996-12003 (1994).

[36] N. Troullier and J. L. Martins. Efficient pseudopotentials for plane-wave calculations. *Physical Review B*, 43:1993-2006 (1991).

[37] M. E. Tuckerman, D. A. Yarne, S. O. Samuelson, A. L. Hughes, and G. J. Martyna. Exploiting multiple levels of parallelism in molecular dynamics based calculations via modern techniques and software paradigms on distributed memory computers. *Computer Physics Communications*, 128:333-376 (2000).

[38] P. Vashishta, R. K. Kalia, and A. Nakano. Large-scale atomistic simulation of dynamic fracture. *Computing in Science & Engineering*, 1(5):56-65 (1999).

[39] M. S. Warren and J. K. Salmon. A portable parallel particle program. *Computer Physics Communications*, 87:266-290 (1995).

[40] D.-Y. Yang, A. Grama, and V. Sarin. Bounded-error compression of particle data from hierarchical approximation methods. In *Proceedings of SC99*. ACM/IEEE, 1999.