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processor of a CRAY Y-MP. As mentioned earlier, the KKR-CPA code has recently been modified so that its parallelism can be exploited over a network of workstations by using PVM. By linking six IBM model 530s and four IBM model 320s together into a parallel virtual machine, the KKR-CPA code is able to execute at about 200 megaflops, which is quite competitive with a single processor of a CRAY Y-MP. The price/performance rate of this PVM configuration is almost 1300 megaflops per $1 million.

The portability and performance of the KKR-CPA code have significantly enhanced the productivity of the materials scientists involved in this project. Excited about the power of parallel processing, researchers at ORNL are beginning computational experiments to address unanswered questions in materials science, and superconductivity in particular.

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Besides the authors, several other researchers have made significant contributions to the development of the KKR-CPA code. Walter Temmerman and Zidka Szotek from SERC Daresbury developed the Cray multitasking routines. Frank Pinski from the University of Cincinnati collaborated on the development of the serial algorithm and code. A. Barbieri at the University of Bristol also participated in the early development of the code.

in excess of 3 gigaflops during the superconductor computations.

The KKR-CPA code calls the BLAS routine ZAXPY in the matrix formation and inversion routines, and an available assembly language version of ZAXPY was linked in. No other complex double-precision BLAS routines were available for the i860 at the time of these studies. Nevertheless, Level 2 BLAS versions of these two KKR-CPA routines have been written and are used when running on all the other computers. Using the BLAS-2 versions, one processor of a CRAY Y-MP performs the matrix inversions at a rate of 302 megaflops and the matrix formation at 300 megaflops. Note in Table 1 that a CRAY Y-MP/8 is capable of rates approaching 2.3 gigaflops when executing the KKR-CPA code.

Table 1 gives the overall performance of the KKR-CPA code on various computers and their cost. Figure 3 shows the price/performance rates for the most cost-effective computers on which the KKR-CPA code is executed.

When using all 128 processors of the Intel iPSC/860, the KKR-CPA code runs at a sustained average rate of 2527 megaflops. The list price for the 128 node Intel iPSC/860 with the CFS configuration that exists at ORNL is $3 million. Given these figures, the price performance of the KKR-CPA code on the Intel machine is 842 megaflops per $1 million.

The full computational analysis of the perovskite superconductors is not viable on a single IBM model 320 because it would require several days. Typical production runs of the KKR-CPA code are done on 64 or 32 nodes of the Intel iPSC/860 or a single

Having made this change, we measured the startup overhead to be less than 0.4% of the total time for the perovskite computations.

In addition to the startup overhead, three computational rate measurements were made on small test runs. First, the average computational rate of each node of the iPSC/860 was measured by having a single node solve ten representative "energy" tasks. The test run was constructed to involve approximately the same amount of communication overhead and file I/O on a per-node basis as for a larger problem. This test run required $3.09 \text{x} 10^{11}$ double-precision floating point operations that were completed in 15,530 seconds. This corresponds to an average rate of 19.9 megaflops per processor. Second, the most computationally intensive step in the algorithm is inverting 160x160 dense double-precision complex matrices. Hundreds of these inversions are performed in each "energy" task, consuming about 78% of the total execution time as measured by HPM. The rate for a single matrix inversion was measured as follows. The number of floating point operations required to invert an $n \text{x} n$ matrix is given by $8n^2(n+1) + 8n^2 + 11n$, where the complex operation $y = y + \alpha x$ takes eight floating point operations. The time per inversion, averaged over 100 inversions, is 1574 ms. The rate for these inversions is thus 21.07 megaflops on an iPSC/860 node. Third, the next most expensive step in the KKR-CPA algorithm is the formation of the matrices to be inverted. HPM reported that about 12% of the total time is spent in these computations, which have been measured at 24.12 megaflops on an iPSC/860 node. Thus, for about 12% of the time the code is executing

material. Details of these findings can be found in [5].

4 Performance results

Computational rates were measured during calculations of the electronic structure of the high-temperature superconductor $(Ba_{1-x}K_x)BiO_3$. The overall computational rate was measured in the following conservative manner. The Cray Hardware Performance Monitor (HPM) was used to count the actual number of double-precision floating point operations in a serial run. This same operation count was used for determining the computational rates of the parallel runs. This was to eliminate any bias in doing more work in the parallel cases to get higher megaflop rates.

Wall clock time, as reported by the UNIX *time* command, was used to determine the number of seconds an application ran. On the Intel machine the total time included the time to load the problem onto 128 nodes, all communication, file I/O (about 2 megabytes of information is read in and about 150 Kbytes is written out), and dynamic load balancing overhead. The largest computational problem ran for 4 1/2 hours on 128 processors of an Intel iPSC/860 and involved 3.92×10^{13} double-precision floating point operations.

To reduce the startup overhead, the large input files were stored on the Intel Concurrent File System (CFS) rather than on an NFS file server. The CFS system at ORNL can read files at an aggregate rate approaching 3 megabytes per second. This did not involve changing any source code, only the storage location of the input files.

temperature of 13 Kelvin. When $BaBiO_3$ is alloyed with potassium, there is substitutional disorder on the barium sublattice, and the material $(Ba_{.6}K_{.4})BiO_3$ has a maximum superconducting transition temperature of 30 Kelvin. One aspect of the KKR-CPA computations was to observe the similarities and differences in the electronic structure of the potassium and lead alloys.

$(Ba_{.6}K_{.4})BiO_3$, shown in Figure 1, has three properties that make it an ideal material to study. First, its perovskite structure contains only five simple cubic sublattices. The bismuth and three oxygen sublattices are ordered, and the sublattice containing a mixture of barium and potassium is disorded. Second, it has a cubic symmetry that can be exploited to reduce the amount of computations required. In particular, integrations over a symmetric cubic cell can be reduced to integrations over the unique 1/48th of the cell. Third, this material falls into the same class of materials (according to Villars' classification [7]) as the yttrium- and lanthanum-based superconductors, which have received so much attention. If it is true that all the materials in each class exhibit superconductivity for similar reasons, it makes sense to try to analyze the simplest materials in the class.

The computational results from the KKR-CPA code showed the effect of alloying on the density of states for this material. These results are shown in Figure 2. The KKR-CPA calculations also produced some new results on fermi-surface nesting that imply the existence of a charge-density wave in this superconductor. This could explain previously puzzling experimental data from electron scattering studies of this

[10]. PVM is composed of a suite of user-interface primitives and supporting software that together enable concurrent computing on loosely coupled heterogeneous networks containing serial and parallel computers. PVM allows tasks to be initiated on machines on the network and for message passing and synchronization between these tasks. Thus it will soon be possible to combine several parallel supercomputers to solve one large computational grand challenge problem. The PVM result is included here to show the future potential of such systems to achieve high performance. In our experiments using PVM, ten IBM RS/6000 workstations worked in parallel to solve the electronic structure calculations. Six model 530s and four model 320s were available for these tests, which were run at night to reduce load imbalances caused by multiple users on these machines.

3 Computational results

The new complex lattice KKR-CPA code has been used to study the electronic structure of several materials, including nickel aluminide, which is a new high-strength alloy being studied at Oak Ridge National Laboratory; MnO, which is a transition metal oxide that is close to the metal/insulator transition; and various alloys of the perovskite material $BaBiO_3$. $BaBiO_3$ has an interesting property: It becomes a high-temperature superconductor if it is alloyed with either potassium or lead. When $BaBiO_3$ is alloyed with lead, there is substitutional disorder on the bismuth sublattice, and the material $Ba(Bi_{.3}Pb_{.7})O_3$ has a maximum superconducting transition

processor is requested, a pool-of-tasks scheme is used for dynamic load balancing. In this scheme the tasks are arranged in a queue in approximate order of decreasing difficulty and assigned to idle slave processors as they become available. Thus all processors are busy as long as there are tasks in the queue. If multitasking is specified in the input file, then a subroutine is called that multitasks the queue of energies on a CRAY Y-MP. If multiple processors are requested, but multitasking is not, then a subroutine is called that manages the queue of tasks through message passing.

Parallelizing over the energies requires an initially high communication overhead as approximately 5 megabytes of data is broadcast to all the processors, but this one-time cost is small compared to the several hours of computation that follows. Every few minutes during the computation partial results amounting to about 100 kilobytes of data is also transfered between master and slave. Because of the high computation to communication ratio and the dynamic load balancing the efficiency of the parallel implementation was measured to be greater than 99%.

This version of the KKR-CPA code consists of approximately 16,000 lines of Fortran divided among 127 subroutines. Only about 20 subroutines are explicitly involved in the parallelization. There are no special assembly language routines, but two subroutines make calls to BLAS routines [4]. On each machine the BLAS library was linked in if it was available.

The KKR-CPA code has also been modified to allow the message-passing subroutines to operate over a network of computers by using PVM (parallel virtual machine)

is the spatial domain under investigation after this domain has been converted to reciprocal space.) Each location was evaluated in terms of the available parallelism and the required communication overhead incurred by splitting the algorithm at that point. The Brillouin zone integration is the main step in each CPA iteration. The disadvantage of parallelizing the Brillouin zone integration is the large volume of communication required. For this reason the integration over energy was parallelized. Typically, this integration involves the evaluation of the single-site Green's function for between 200 and 1000 energies in order to determine the charge density for the next self-consistency iteration. Each of these tasks involves the iterative solution of the CPA equations for the given energy and requires significantly more computation than communication.

The parallel implementation is based on a master/slave paradigm to reduce memory requirements and synchronization overhead. In our implementation one processor is responsible for reading the main input file, which contains the number of processors to be used, the problem description, and the location of relevant data files. This master processor also manages the LDA-DFT charge self-consistency iteration. The slave processors require only enough memory to solve the CPA equations for a single energy, which presently requires 7 megabytes. Memory reduction was a crucial consideration for porting the KKR-CPA code to the Intel iPSC/860 because the individual nodes contain only 8 megabytes of RAM. If only one processor is requested, then a subroutine is called that calculates the tasks serially. When more than one

Cray machines at the National Energy Research Supercomputer Center at Lawrence Livermore National Laboratory, the State of Ohio Supercomputer Center, and the Rutherford Laboratory in the United Kingdom. However, the computational performance of the code was found to be inadequate to analyze the new superconductors.

The next section discusses the efforts to incorporate parallelization into the KKR-CPA code while still maintaining its portability and generality. The final sections describe the high performance obtained with the new version of the code and some new insights into the electronic structure of a perovskite superconductor.

2 Parallelization

To exploit the emerging power of parallel processors, we redesigned the KKR-CPA code to allow the same source code to execute efficiently on serial computers, on a shared-memory multiprocessor (CRAY Y-MP), and on a distributed-memory multiprocessor (Intel iPSC/860). This section describes the techniques used to achieve this result.

The KKR-CPA algorithm contains several locations where parallelism can be exploited. These locations correspond to integrations in the KKR-CPA algorithm. Evaluating integrals typically involves the independent evaluation of a function at different locations and the merging of these data into a final value. The two most obvious locations for parallelization in the KKR-CPA algorithm are in the integration over the Brillouin zone and the integration over energy. (The Brillouin zone

The motivations for the development of the multi-sublattice KKR-CPA code described in this paper are diverse, ranging from applied alloy design efforts to fundamental questions regarding compositional, magnetic, and other fluctuations that occur in materials away from absolute zero temperature. Not least of the motivating factors was the 1986 discovery of a new class of high-temperature superconducting ceramic-based materials. This discovery has led to an intense research effort to understand the source of high-temperature superconductivity. Such an understanding would be an important step toward the development of practical devices such as ultrasensitive scientific instruments, high-speed computers, and powerful magnets. A great deal of computational effort has been expended in analyzing these materials.

Most of the high-temperature superconductors are disordered either because of alloying or because of oxygen nonstoichiometry. Thus a method for studying the effects of alloying disorder on the electronic structure of these materials is needed. Also, because the high-temperature superconductors are derived from materials that are on the borderline between metal and insulator, questions about the applicability of LDA-DFT in general are raised because standard LDA-DFT fails to adequately describe the electronic properties of materials that are close to the metal/insulator transition. The KKR-CPA algorithm is well suited to analyzing several properties of these materials.

The multi-sublattice KKR-CPA algorithm has been developed into a general application code written entirely in Fortran 77. Production runs were initially made on

that are measured experimentally. The complex task of configurational averaging is accomplished by the coherent potential approximation (CPA), which is a mean field treatment of the effects of disorder and yields the conditionally averaged Green's function, charge density, and so on. The conditional average is defined such that the atomic species at a site is specified and the occupancy of all other sites is averaged over. Within LDA-DFT it is the conditionally averaged single-site charge density that is made self-consistent with the configurationally averaged single-site effective potential. In simple single-sublattice systems such as fcc and bcc alloys, the KKR-CPA method has proved very successful for describing the effects of disorder on the physical and metallurgical properties of alloys.

As in typical mean-field theories, the averaging process implicit in the CPA involves the self-consistent solution of a set of integral equations. In the KKR-CPA method these equations are formulated within a multiple-scattering Green's function framework. The central issue is that the effects of disorder on the electronic structure are modeled through the scattering properties of some effective scatterer (or single-site coherent potential) that is the same on every site in the crystal. The properties of the effective scatterer are determined such that an ordered periodic array of these effective scatterers gives the "best" representation of the scattering properties of the original nonperiodic disordered array of scatterers. The CPA algorithm calculates the "best" effective scatterer that can be obtained using only conditionally averaged single-site quantities.

The theoretical background for the KKR-CPA method is provided by the local density approximation to density functional theory (LDA-DFT) [9]. The fundamental result of density functional theory is that the ground state energy of any system of electrons and nuclei is a unique functional of the electron density. Moreover, this electron density can be obtained by solving a set of self-consistent field equations for the motion of a single electron in the presence of an effective field generated by the nuclei and other electrons. The complex many-electron exchange and correlation effects are handled through an effective exchange-correlation potential that is explicitly added to the potential energy term in Schrödinger's equation. Since this exchange-correlation potential is not exactly known for the interacting inhomogeneous electron charge distribution appropriate to condensed matter, it is often approximated point by point in space by the charge distribution for a homogeneous interacting electron gas having the density at that point. While not exact, this local density approximation has proved to be a powerful device for practical calculations of the properties of a wide range of metals, alloys, semiconductors, and other materials.

The KKR-CPA method extends the usual implementation of LDA-DFT theory to substitutionally disordered materials [3]. In this sense it is a completely first-principles theory of the properties of substitutionally disordered materials requiring as input only the atomic numbers of the species making up the solid. The KKR-CPA method yields the configurationally averaged Green's function, charge density, energy, and other properties directly. It is the configurationally averaged properties

and potentials that can be used to compute the response of the material to many perturbations. One important perturbation is the potential shift of phase of an alloy due to a small change of concentration of one of its component atoms. Such materials are thought to be important in the design of "smart" materials that change shape or stiffness in response to outside forces.

During the last few years Oak Ridge National Laboratory (ORNL) material scientists and their collaborators at the University of Cincinnati, Science and Engineering Research Council (SERC) at Daresbury, and the University of Bristol have been developing an algorithm for studying the physical properties of complex substitutionally disordered materials. A few important examples of physical systems and situations in which substitutional disorder plays a critical role in determining material properties include metallic alloys, high-temperature superconductors, magnetic phase transitions, and metal/insulator transitions. The algorithm being developed is an implementation of the Korringa, Kohn, and Rostoker coherent potential approximation (KKR-CPA) method for calculating the electronic properties, energetics, and other ground state properties of substitutionally disordered alloys [2,6,8]. The implementation treats materials with complex atomic lattices and any number of disordered sublattices. The algorithm also solves the underlying quantum mechanical equations within a fully relativistic framework [1]. This is necessary for materials containing heavy elements such as barium in which even the outer, bonding, electrons are travelling at a significant fraction of the velocity of light.

Abstract

Researchers at Oak Ridge National Laboratory have developed an application code for calculating the electronic properties and energetics of disordered materials. The same source code has been compiled and run on workstations, Crays, and the Intel iPSC/860. This electronic structures code is capable of running at over 2 gigaflops on both an 8-processor CRAY Y-MP and a 128-processor Intel iPSC/860.

Using this new KKR-CPA code, we executed density-of-state computations of a perovskite superconductor at a rate of 2527 megaflops on the Intel iPSC/860. This corresponds to a price/performance rate of 842 megaflops per $1 million based on the list price of this computer. Similar but smaller computations done on a network of ten IBM RS/6000 workstations executed at a price/performance rate of 1.3 gigaflops per $1 million.

1 Introduction

Computational simulation and analysis of materials with supercomputers has emerged as an important conponent in the design of new materials. Traditional research in laboratories is now being enhanced by discoveries made on high-performance computers. Solid state physicists and material scientists study the mutual forces of attraction and repulsion among atoms in a material and concentrate on understanding the fundamental properties of matter. They are interested in the calculation of the quantum mechanical ground state of complex materials. This calculation yields wavefunctions

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Parallel Superconductor Code

on the iPSC/860