Itanium®-based System Powers 100X Improvement in Scientific Computation

THE UNIVERSITY OF
WARWICK

Centre for Scientific Computing

"To go to even larger-scale applications, we had to turn to the 64-bit Itanium processors. All parts of the method were adapted to the full 64-bit architecture, so we could use all the processor facilities and maximize performance."

– Dr. Rudolf A. Roemer, University of Warwick, Centre for Scientific Computing

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COMPUTATIONALLY
INTENSIVE

One of the toughest challenges in modern scientific computation is the numerical solution of large-scale quantum problems arising from the physics of disordered systems. These problems commonly involve the calculation of eigenvalues and eigenvectors – mathematical entities used to describe the energies and spatial distribution of charged particles, for example. These calculations may often expand to the simultaneous solution of several million equations with several million unknowns.

At the Centre for Scientific Computing at the University of Warwick, an international team of scientists has demonstrated a greatly improved computational approach for these types of calculations, using an important and common scientific problem: finding eigenvalues and eigenvectors of large, sparse, symmetric and highly indefinite matrices. These matrices may contain as many as hundreds of millions of rows and columns, making the calculation of a solution impossible only a few years ago.

Using an SGI Altix* supercomputer running Intel® Itanium® processors, the team developed computational improvements that boost performance by orders of magnitude over previous approaches, while also optimizing memory requirements. To prove their approach, they calculated a 3D map of electron distribution within a material in just three days, 100 times faster than previous attempts.

ITANIUM®SOLUTIONS
A L L I A N C E

Challenge

The numerical solution of large-scale eigenvalue problems is a common problem in quantum physics, exemplified by the Anderson model of localization. This model is important for a wide range of applications, including research in amorphous alloys, semiconductors and DNA. In addition to several million unknowns, these models use underlying structure involving random perturbations that prevent the use of simple preconditioning approaches to simplify the calculations.

To circumvent this problem, the team evaluated how to apply new preconditioning approaches for symmetric, indefinite linear systems and eigenvalue problems with the Anderson model. The team chose two modern eigenvalue solver strategies: Pardiso, a direct solver which includes a "shift-and-invert" technique, and iterative approaches such as Arpack or JDBSym in combination with the Ilupack factorization package. By combining and modifying these solvers, the team created an extremely efficient preconditioner for the Anderson model that is memory efficient while at the same time accelerates the eigenvalue computations. Optimized for the 64-bit Itanium®-based platform, the resulting solution can calculate interior eigenvalues and eigenvectors for an Anderson model several orders of magnitudes faster than traditional algorithms without similar increases in memory requirements.
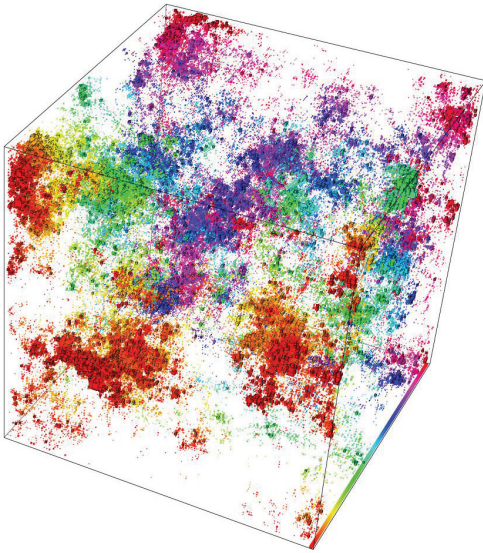
A wave function probability for the 3D Anderson Model of localization with atoms.

Results

The performance increase of the new and improved algorithms, combined with the speed of the Itanium®-based supercomputer, makes it possible to solve a class of problems quickly and easily which have until recently been considered far too large. This approach requires only a moderate amount of memory, thus allowing scientists to study the Anderson eigenproblem on significantly larger scales than ever before. For example, it is possible to solve N x N matrices as large as $N = 64 \cdot 10^6$ columns and rows in just a few days.

Roughly two years after starting the development of this approach on the Itanium-based Altix supercomputer, the team delivered the world's largest and most detailed 3D map of the distribution of an electron over a lattice of 42 million atoms. The final solver package, JADAMILU, used in this algorithmic strategy is now available and already widely used in many high-profile science programs.

The results of the team's work have appeared in several scientific journals, including the paper "On Large Scale Diagonalization Techniques for the Anderson Model of Localization" in the prestigious SIGEST section of the SIAM Reviews Journal. The editors of SIAM explained that: "as large as the increases in computer speed have been, they have been matched by improvements from more efficient algorithms... [this work] is an example of this tremendous type of algorithmic improvement."

It's also a great example of how Itanium-based systems are solving some of the biggest computational problems in science.

System Configuration

Hardware: SGI Altix* 3700/BX2 with 56 Intel® Itanium® 2 processors, 112 GB of main memory.

Operating system: UNIX*

Applications: Executable codes optimized by Intel® V8.1 compiler suite and linked with MKL basic linear algebra subprograms. The sparse direct solver used the OpenMP for parallelization.

Benefits of Itanium

The full 64-bit Intel® Itanium® architecture was critical as the computational requirements of the Anderson model surpassed 32-bit architectures. This includes not only the access of memory but all parts of the method to be adapted to the full 64-bit bandwidth.