Applications with a need for a large shared memory resource

Sven Stafström[1,2], Mikael Unge[1], Torgny Faxen[2], and Patrick Norman[1,2]

[1] Linköping University, NSC, SE-581 83, Linköping, Sweden
sst@ifm.liu.se,
WWW home page:http://www.ifm.liu.se/ svens/
[2] Linköping University, IFM, SE-581 83, Linköping, Sweden

Abstract. The new shared memory system (SMP) at the National Supercomputer Center (NSC) at Linköping University will be presented together with some benchmark results and one application example, which deals with computational materials science. In this application we used the large shared memory resource to generate a set of correlated random numbers that describe imperfections in crystallinde materials. Finite-size scaling, i.e, studies of a sequence of successively larger systems, is used to make predictions concerning the properties of infinite systems. Based on our numerical results we can conclude that a metal-insulator-transition exists in two-dimensional crystalline material with correlated disorder.

1 The SMP system at NSC

NSC recently accuired a large SMP system, a SGI Altix 3700 Bx2 with 64 Intel Itanium 2 processors and 512 GB of memory. The system was financed by the Swedish Research Council via the Swedish National Infrastructure for Computing (SNIC). It is the largest SMP system in Sweden and it is intended to be used a a capability resource for specific memory demanding applications.

2 VASP and Gaussian 03 benchmarks

A user survey among the Swedish high performance computing (HPC) community was carried out during 2005. From this survey it was concluded that the need for a SMP resource in Sweden is large. The most requested application software for calculations requiring a large shared memory turned out to be the quantum chemistry code Gaussian 03[1] and the solid state physics code VASP [2–4]. Some benchmark results for these codes on the Altix system will be presented.

3 Application example: Finite-size scaling

Since the discovery of the effect of disorder on the electron diffusion properties in solids by Anderson[5] an enormous amount of work has been devoted

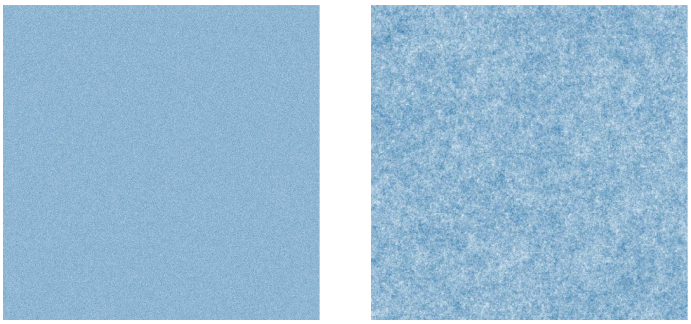
to the relation between material imperfections and their physical properties. In particular, electron transport in doped semi-conductors and later in conjugated polymers and organic materials has been the focus of these studies. The access to high performance computing resources has opened up a possibility to perform numerical investigations on realistic system.

It is suggested that introduction of long-range correlation in the system can yield delocalized states in one and two dimensions [**?**,**?**,**?**,**?**].

We generate the on-site potential energies, ε_i, with a long-range correlation. The long-range correlation correspond to the potential induced by the randomly distributed dipoles [**?**]. For this, we apply the Modified Fourier Filtering Method (MFFM) [**?**]. It consist of filtering the Fourier components of an uncorrelated sequence of random numbers, $\{u_i\}$, with a power law filter, $\varepsilon_{\mathbf{q}} = \sqrt{S(\mathbf{q})}u_{\mathbf{q}}$. The inverse Fourier transform yields a correlated sequence $\{\varepsilon_i\}$. The drawback of the original Fourier Filtering Method (FFM) [**?**,**?**] is that only 1% of the generated numbers in two dimensions has the desired correlation [**?**]. For one dimension this fraction is as low as 0.1% [**?**]. In one dimensional FFM the correlation function is defined as $C_{\mathrm{FFM}}(l) = \langle \varepsilon_i \varepsilon_{i+l} \rangle \sim l^{-\gamma}$. $C_{\mathrm{FFM}}(l)$ has a singularity at $l = 0$, this yields aliasing effects, this destroy the desired correlation. This is avoided in MFFM by modify the correlation function so that it is well defined for $l = 0$,

$$C_{\mathrm{MFFM}}(l) = \langle \varepsilon_i \varepsilon_{i+l} \rangle = (1 + l2)^{-\gamma/2}. \tag{1}$$

Fig. 1 shows a set, 1024×1024, of uncorrelated numbers and correlated counterpart with $\gamma = 1.0$ generated with the two dimensional form of Eqeq:MFFM [**?**]. The largest set of correlated numbers generated is 1024×2^{23}, note that the generation of this set requires $\sim$ 256GB RAM.



a) b)

Fig. 1. Surface plots of square lattices of 1024×1024 uncorrelated numbers, a), and correlated numbers with $\gamma = 1.0$, b).

There is no indication that the localization length for the extended model saturates, rather the opposite. According to finite size scaling this would yield a

MIT [**?**]. To show that calculations for larger N are needed. However, our results do show a substantial increase in the localization length of the electronic state in pentacene with correlated disordered as compared to the case of uncorrelated disorder.

In conclusion, the results presented here show that molecular crystals such as pentacene can exhibit extended states only if there exist correlation in the static disorder. The existence of this type of disorder is supported by the experimental result of bandlike transport of single crystals of pentacene at room temperature [**?**].

References

1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople. Gaussian 03, Revision C.02. Gaussian, Inc., Wallingford, CT, 2004.
2. G. Kresse and J. Hafner: *Ab initio* molecular dynamics for liquid metals Phys. Rev. B **47** (1993) 558.
3. G. Kresse and J. Furthmüller: Comput. Mater. Sci. **6** (1996) 15.
4. G. Kresse and J. Furthmüller: Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set Phys. Rev. B **54** (1996) 11169.
5. P. W. Anderson: Absence of diffusion in certain random lattices Phys. Rev. **109**, (1958) 1492-1505.