

Extending the domain of quantum mechanical simulations with HPCx



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Eighteen years ago the computational physics community was shaken by the seminal work of Car and Parrinello, who introduced the idea of first principles molecular dynamics, i.e. moving the atoms of a real system using quantum mechanics forces. Their idea was so powerful and forward looking that it spread widely, even crossing the boundary of computational physics, and nowadays similar techniques are used in a wide range of disciplines, including chemistry, geophysics and biology. In 1985 Car and Parrinello were able to calculate the frequency of a chosen mode of vibration of a silicon crystal by simulating the motion of a system containing 8 atoms of silicon for a fraction of a picosecond. Since then, computers have multiplied their capabilities, codes have improved, and the frontiers have been regularly pushed forward, so that now simulations on ~100 atoms for ~1-10 ps are routinely carried out.

The advent of HPCx represents one of these moments in which previous boundaries can be extended. In this short article I report the first quantum mechanics simulation of direct coexistence of solids and liquids.

Using molecular dynamics based on density functional theory I have simulated a 1000 atoms system of solid and liquid aluminium in coexistence for 15 ps (a snapshot of this simulation is displayed in Fig. 1). From these simulations I have extracted points on the melting curve of aluminium reported in Fig. 2. At the same time, I have also simulated a few 512 atoms systems for 40 ps; the points on the melting curve extracted using these simulations are also reported in Fig. 2. The difference between the results obtained with 512 and 1000 atoms suggests that 512 atoms are probably still not enough for this type or problem, hence the necessity of a powerful supercomputer. In Fig. 2 I also report the melting curve of aluminium calculated previously using different techniques, based on the calculation of the free energies of solid and liquids (L. Vočadlo and D. Alfè, PRB 65, 214105, 2002). Free energies can be calculated on relatively small systems (~100 atoms) by making use of the technique known as thermodynamic integration (see e.g. D. Frenkel and B. Smit, "Understanding molecular simulations", Academic Press, San Diego, 1996), so that this work has been possible on previous generations of supercomputers.

The very good agreement between the two sets of calculations is gratifying, and therefore the two techniques support each other.

This result is extremely important for at least two reasons. The first is that a number of melting properties have been calculated using free energies techniques, and the present findings strongly support the adequacy of those techniques used in the past. The second is related to a shift of paradigm:

coexistence simulations are more easily carried out than free energy calculations, and the main effort is relieved from the human to be relocated on the computer. I believe that in the future we will witness broad applications of these types of simulations.

The present work has only been possible thanks to HPCx, and each simulation has been completed in little over two weeks of continuous running on 128 processors (roughly, half of the machine was dedicated to the running of all these simulations).

The good news is that the HPCx machine has room for improving its performance, which is now hindered by the relatively poor inter-boxes communications. This creates serious problems for those codes that move large amount of data among the processors, like electronic structure programs. It is also somewhat unfortunate that the machine has been configured in a way that makes this problem even worse: with the partitioning of the machine in logical partitions (LPA) of 8 nodes each, one can only be sure or running inside one box if the number of required processors is less or equal to 8. In my opinion, it would be desirable to have the possibility of running inside a whole box of 32 processors.

(Editor's note: The phase 2 HPCx system upgrades, operational in the second half of 2004, are specifically designed to address these two issues.)

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Dario's paper can be found here:
www.hpcx.ac.uk/research/publications/al_coex.pdf

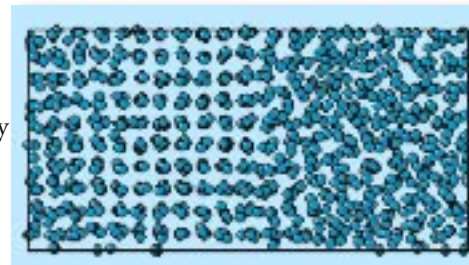


Fig. 1. First principles simulation of solid and liquid aluminium in coexistence. The simulation lasts for 15 ps and the cell contains 1000 atoms.

Fig. 2. Melting points of aluminium calculated using the method of the coexistence of phases: points from 1000 atoms simulations and triangles from 512 atoms simulations. The continuous line represents previous results with errors (dashed lines) obtained using the free energy approach (Vočadlo and Alfè 2002).

