The IEEE Computer Society and iVEC invite you to a supercomputing seminar:

Quantum-chemistry simulation at the petascale level: a new parallelisation approach

Simulating complex materials and biological systems is a big challenge despite the availability of supercomputers. To support the complexity of research simulations, code needs to be scaled to utilise thousands of CPUs. In some cases of biological research it is simply impossible to simulate the systems without thousands of CPUs, so these are typically situations in which petascale hardware makes the difference between doing or not doing a particular kind of research. One of the most promising techniques used for studying the properties of these systems is based on Density Functional Theory (DFT) approach and its extension.

This technique is widely used in solid state physics where the sample is usually periodic. Unfortunately, disordered solids and biophysical systems cannot be treated by using this assumption so a large supercell is necessary. This talk presents a new parallelisation approach aimed to overcome the limit of the traditional parallelisation approach in plane-waves DFT codes. In the framework of the Partnership for Advanced Computing in Europe (PRACE) Implementation Phases I&II, a new parallelisation strategy over the electronic bands has been introduced.

In order to show the efficacy of this approach, two challenging kernels has been identified: the linear response (used to compute NMR spectra) and the Exact-Exchange (to evaluate the Fock exchange operator, in hybrid-DFT functionals). These two kernels are well isolated inside the Quantum-ESPRESSO (opEn-Source Package for Research in Electronic Structure, Simulation, and Optimisation) distribution, and are constituted by several nested loops. Moreover, they are very time consuming: any scalability improvements are going to have a significant, positive effect on execution time.

The benchmark results reported in this talk will prove that this parallelisation approach achieves good scaling on many thousands of CPUs, and spreads the band parallelization to the whole Quantum-ESPRESSO package. This strategy is a breakthrough in plane-waves DFT codes, allowing them to fully exploit petascale hardware and beyond.

Presenter: Dr Nicola Varini, iVEC Supercomputing Specialist
Venue: ARRC Auditorium, 26 Dick Perry Ave, Kensington
Date: 26th October
Time: 4-5pm, followed by sundowner.
Cost: Free

Please RSVP your attendance to rsvp@ivec.org

iVEC is an unincorporated joint venture of CSIRO and the four public WA universities with funding from the State Government. iVEC fosters and promotes scientific and technological innovation through the provision of supercomputing and eResearch services to the research community, commercial organisations and government agencies. In 2009, iVEC was charged with establishing and operating the $80 million Pawsey Centre by the Australian government.