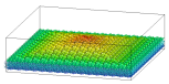
Use of the O(N) ab initio code CONQUEST



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1 Workshop Details

1.1 Details

Timing
Number of days : 2
Start : 2007-09-07
end : 2007-09-08

Location of the activity
CECAM
46 allé e d'Italie
69007 Lyon
France

1.2 Description

No description provided

2 Requested Support

CECAM

Psi-k

3 Participant List

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4 Organizer’s report

4.1 Conclusions.

The Conquest code is mature enough that experienced electronic structure researchers can successfully use it

Challenging applications on large systems are now possible which cannot be reached with standard codes

Direct interaction with developers and experienced users is extremely helpful

The technique is sufficiently different to standard electronic structure codes that a tutorial is an important part of teaching new users

The method introduces new basis sets (local orbitals) as well as linear scaling, which requires teaching in two separate areas

4.2 Recommendations.

The Conquest beta test should be gradually widened, giving more groups access to the code

The O(N) field needs more users and developers to realise the potential inherent in the techniques

Interaction with the developers through on-line forums, email lists and tutorial/workshops should be maximised

More Conquest tutorials should be planned to help speed the increased use of the code

Tutorials on local orbital methods could be organised jointly with other European groups such as SIESTA, as well as the joint workshops which have been so successful

5 Key references

[1] D. R. Bowler and R. Choudhury and M. J. Gillan and T. Miyazaki *Recent progress with large-scale ab initio calculations: the CONQUEST code*, phys. stat. sol. b **243** 989-1000 (2006)

[2] T. Miyazaki and D. R. Bowler and R. Choudhury andM. J. Gillan *Atomic force algorithms in density functional theory electronic-structure techniques based on local orbitals*, Journal of Chemical Physics **121** 6186-6194 (2004)

[3] D. R. Bowler and T. Miyazaki and M. J. Gillan *Recent progress in linear scaling ab initio electronic structure techniques*, Journal of Physics: Condensed Matter **14** 2781-2798 (2002)

[4] Full details can be found on the Conquest web page , http://www.conquest.ucl.ac.uk/ ()