

High performance density functional theory: Wavelets, order(N) scaling, parallelism

Tutorial BigDFT - Nov 26 to Nov 30 2007

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Monday: DFT and its mystery

- 9:00 - 9:10 Welcome & practical details
- 9:10 - 10:00 Basics of DFT
Kohn-Sham equations
- 10:00 - 10:30 Coffee break
- 10:30 - 12:30 Operations used in DFT-Kohn-Sham
with applications to plane waves
- 12:30 - 14:30 Lunch
- 14:30 - 15:00 Gaussian basis sets
- 15:00 - 15:00 Coffee break
- 15:30 - 16:30 Overview of physical properties
accessible by DFT Kohn-Sham
- 16:30 - 18:00 Exercises: ABINIT Tutorial 1 and 2

Tuesday: Mathematics of wavelets

- 9:00 - 9:10 Welcome & practical details.
- 9:10 - 10:00 Introduction to multi-resolution analysis
- 10:00 - 10:30 Coffee break
- 10:30 - 12:30 Daubechies wavelets and
interpolating scaling functions:
PDE and kinetic operator
- 12:30 - 14:30 Lunch
- 14:30 - 15:30 Accuracy, convergence and adaptivity
- 15:30 - 18:00 Exercises: wavelet transforms

Wednesday: Inside BigDFT (Machinery)

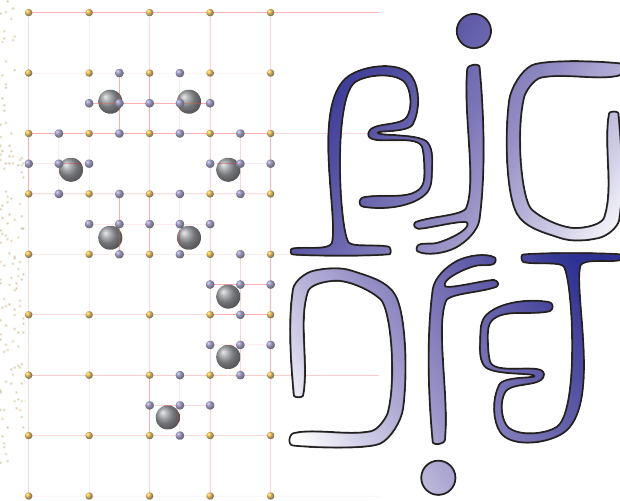
- 9:00 - 9:10 Welcome & practical details.
- 9:10 - 10:00 Data representations, structures,
integration in ABINIT, parallelisation
- 10:00 - 10:30 Coffee break
- 10:30 - 12:30 Convolutions, local potential, preconditioner
- 12:30 - 14:30 Lunch
- 14:30 - 15:30 Poisson solver (isolated, surface),
non-local pseudopotentials, atomic forces
- 15:30 - 18:00 Exercises: Poisson solver,
ABINIT-wavelet
- 20:00 Social Dinner (restaurant les Lyonnais, Vieux Lyon)

Thursday: $O(N)$ method and performances

- 9:00 - 9:10 Welcome & practical details.
- 9:10 - 11:00 Fundamentals of linear scaling methods
- 11:00 - 11:30 Coffee break
- 11:30 - 12:15 Order N in BigDFT, parallelisation
- 12:15 - 14:15 Lunch
- 14:15 - 14:45 Performances
- 14:45 - 15:15 Coffe break
- 15:15 - 18:00 Exercises: $O(N)$,
tests, performances

Friday: Parallelisation, Perspectives

- 9:00 - 9:10 Welcome & practical details.
- 9:10 - 10:00 Planned developments
- 10:00 - 10:30 Coffee break
- 10:30 - 12:30 Exercises: Parallelisation



abinit.org