Introduction to ONETEP

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Outline

• Overview of basic concepts
  – OBDMM approaches
  – NGWFS, density kernel
  – Psinc basis set
  – FFT box
  – Linear-scaling examples
  – Parallel scaling

• Functionality available
• Compilation requirements
• Running a simple calculation
Optimal basis density matrix minimization (OBDMM) approaches
(S. Goedecker, Rev. Mod. Phys., 71, 1085 (1999))


Efficient linear-scaling:

• Use a small basis set of localised non-orthogonal functions to express all quantities to obtain sparse matrices (e.g. Hamiltonian matrix, overlap matrix, etc) with modest memory requirements
• Apply your chosen density matrix minimisation algorithm(s), using efficient sparse matrix algebra techniques

Large basis set accuracy:

• Make sure that the small basis set is “optimal”, by determining it variationally, in situ
• Therefore the small basis set is not fixed (hence it is not a basis set) but it is expressed in terms of a very detailed, highly accurate large basis set
The ONETEP approach

\[ \rho(r, r') = \sum_n f_n \psi_n(r) \psi^*_n(r') \]

**ONETEP** is an **OBDMM** method

- The NGWFs are the “small basis set”
- Each NGWF is expanded in a “large” basis set of psinc functions (this is the actual basis set)

Density matrix localisation

\[ \rho(r, r') = \sum_{\alpha\beta} \phi_\alpha(r) K^{\alpha\beta} \phi_\beta(r') \]

- Impose spatial cut-offs:
  - NGWFs confined to spherical regions
  - Sparse density kernel \( K \) by truncation
NGWF optimisation

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NGWF optimisation

BaTiO₃

Basis set: psinc functions

• “Periodic Cardinal Sine” or Lagrange-mesh functions:
  - Real linear combinations of plane waves
  - Localised
  - Orthogonal

Psinc basis energy cut-off

Basis set variational approaches:

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FFT box technique

simulation cell
FFT box technique

Linear scaling: DNA

Linear-scaling: Amyloid fibrils

Structures of the amyloid fibril kindly provided by the authors of
True linear scaling

Parallel scaling: carbon nanotubes

- 9600 atoms
- Commodity cluster of 24 dual socket dual core Opteron nodes


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Functionality

- LDA (Ceperley-Alder-Perdew-Zunger, Vosko-Wilk-Nusair) and GGAs (Perdew-Wang ’91, Perdew-Burke-Ernzerhof, revPBE, RPBE, BLYP, XLYP)
- Spin polarisation
- Forces
- Geometry optimisation
- Electronic structure analysis
- Visualisation
- Modified Coulomb interactions (Cut-off Coulomb and Martyna-Tuckerman approaches)
Compiling ONETEP

Simple multi-platform build system, needs:

• Fortran 95 compiler
• BLAS and LAPACK numerical libraries
• FFT library: vendor-supplied or FFTw
  – www.fftw.org
• MPI library for parallel version
  – www.lam-mpi.org
Running ONETEP

• Parallel computer
  – Minimum 2 GB per processor (core)
  – Typically distribute 10-100 atoms per processor
  – Cross-over >100 atoms

• Prepare input file: free format
  – Documentation at www.onetep.org

• Supply pseudopotential files (.recpot format)
Input file

• Keywords of different types:
  – Integer
  – Boolean
  – String
  – Real
  – Physical (real + unit)
  – Block data e.g. atomic positions, delimited by `%block` and `%endblock`

• Atomic units by default (hartree and bohr)
• Beware older keywords e.g. `kernel_cutoff`
Example input file: formaldehyde

! Example input file for the ONETEP program
! Formaldehyde molecule

cutoff_energy 600 eV

%block lattice_cart
  48.00  0.00  0.00
  0.00  48.00  0.00
  0.00  0.00  48.00
%endblock lattice_cart

%block positions_abs
  O  24.887507  23.896975  22.647313
  C  27.731659  23.667449  22.643306
  H  28.655157  21.721170  22.637547
  H  28.955467  25.440371  22.646039
%endblock positions_abs

%block species
  O  O  8  4  6.5
  C  C  6  4  6.5
  H  H  1  1  6.5
%endblock species

%block species_pot
  O  oxygen.recpot
  C  carbon.recpot
  H  hydrogen.recpot
%endblock species_pot

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ONETEP calculation outline

• Initialisation phase:
  – Construct initial NGWFs (STOs or PAOs)
  – Construct initial charge density (atomic superposition) and effective potential
  – Construct initial Hamiltonian
  – Obtain initial (non-self-consistent) density kernel using canonical purification
  – Refine initial density kernel (self-consistently) using penalty functional
ONETEP calculation outline continued

• Main optimisation phase:
  – Combination of nested self-consistent loops
  – Outer loop optimises the NGWFs (density kernel fixed)
  – Inner loop optimises the density kernel (NGWFs fixed) using DMM approaches

• Final analysis phase:
  – Calculate forces
  – Write out potentials, densities, NGWFs for plotting
  – Mulliken population analysis
  – Diagonalisation yields wave functions, DOS etc.
Example output file: formaldehyde

View h2co.out
More information

• www.onetep.org

• Scientific highlight of the month:
  – $\Psi_k$ Newsletter 72, December 2005
  – http://psi-k.dl.ac.uk/