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CP2K: Recent performance improvements and new TD-DFT functionality

ARCHER Virtual Tutorial, 23rd Nov 2016

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Reusing this material

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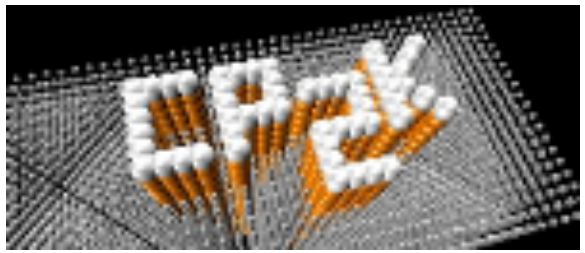
Outline

- CP2K 4.1 Release
- Performance Improvements
  - eCSE 06-06 (Iain Bethune & Mark Tucker, EPCC)
- Time Dependent DFT functionality
  - eCSE 03-11 (Matt Watkins & Sergey Chulkov, University of Lincoln)

CP2K Overview

"CP2K is a program to perform atomistic and molecular simulations of solid state, liquid, molecular, and biological systems. It provides a general framework for different methods such as e.g., density functional theory (DFT) using a mixed Gaussian and plane waves approach (GPW) and classical pair and many-body potentials."

From www.cp2k.org (2004!)



2nd most heavily used code on ARCHER, >2000 MAU since 2014

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CP2K Overview

- Many force models:
  - Classical
  - DFT (GPW, GAPW + vDW)
  - Hybrid Hartree-Fock
  - LS-DFT
  - post-HF (MP2, RPA)
  - Combinations (QM/MM, mixed)
- Simulation tools
  - MD (various ensembles)
  - Monte Carlo
  - Minimisation (GEO/CELL_OPT)
  - Properties (Spectra, excitations …)
- Open Source
  - GPL, www.cp2k.org
  - 1m loc, ~2 commits per day
  - ~20 core developers

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CP2K 4.1

- Released 5th Oct 2016
  - Installed on ARCHER 19th October

https://www.archer.ac.uk/documentation/software/cp2k/ for documentation, benchmarks, hints and tips…

  - Default version:

```
module load cp2k
```

Previous releases also available:

```
module load cp2k/3.0.16521
module load cp2k/2.7.15791
```

- New features
  - Modified Atomic Orbitals analysis (Heinzmann & Alrichs, 1976)
  - Interface to OMEN for NEGF transport calculations
  - Linear Scaling DFT
    - Polarized Atomic Orbitals (Berghold *et al*, 2002)
    - Curvy Steps (Shao *et al*, 2003)
  - O(N^3) RPA implementation
  - k-Points improvements (https://www.cp2k.org/faq:kpoints)
  - TD-DFT with Hybrid Functionals (more later)

Complete list:
https://www.cp2k.org/version_history

CP2K Training

- CP2K User Group Meeting
  - Monday 9th Jan 2017
  - In Edinburgh (travel funding available for UK users)
  - Keynote speaker - Prof. Jürg Hutter, University of Zurich
  - Method & application talks
  - Lightning talks

  - Info from last year: https://www.epcc.ed.ac.uk/content/cp2k-uk-workshop-2016

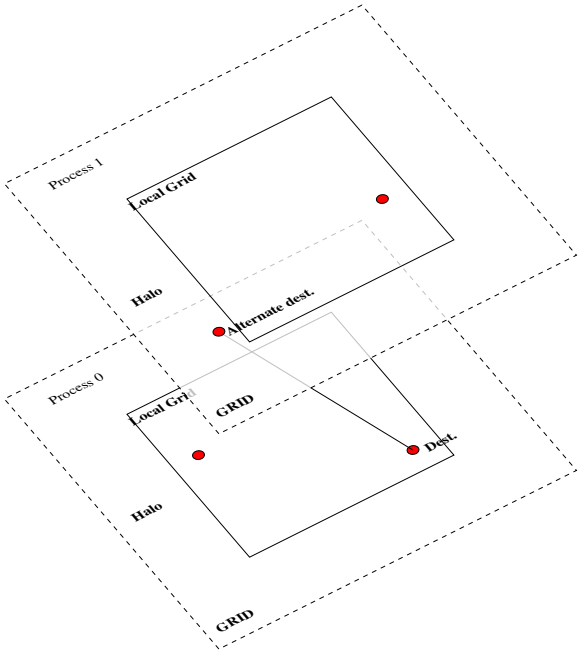
- Hands-on CP2K training / development support
  - Contact ibethune@epcc.ed.ac.uk

Performance Improvements

- Load balancing for disordered / inhomogeneous systems

- Existing algorithm:
  - Serial, $O(p^2)$ memory and time
  - Disabled for p > 1024

- New algorithm:
  - MPI parallel, O(p) memory and time
  - Uses MPI_Scan()
  - Enabled by default



From P. Shivadasan, MSc Thesis, 2014

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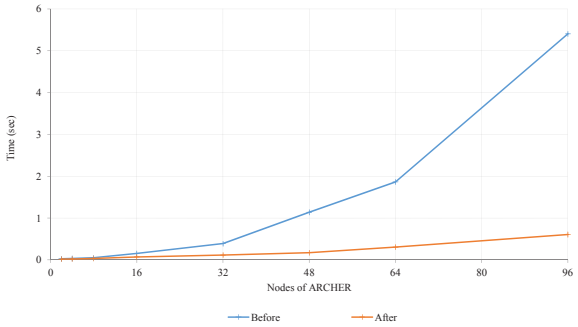
Performance Improvements

Nodes of ARCHER	2	4	8	16	32	48	64	96
Old Algorithm (millisec)	26	32	51	153	389	1140	1864	5406
New Algorithm (millisec)	17	20	34	69	115	171	305	607
Speedup	1.53	1.60	1.50	2.22	3.38	6.67	6.11	8.91

Table 1: Time in `optimize_load_list`



Saving 3.3GB memory per node

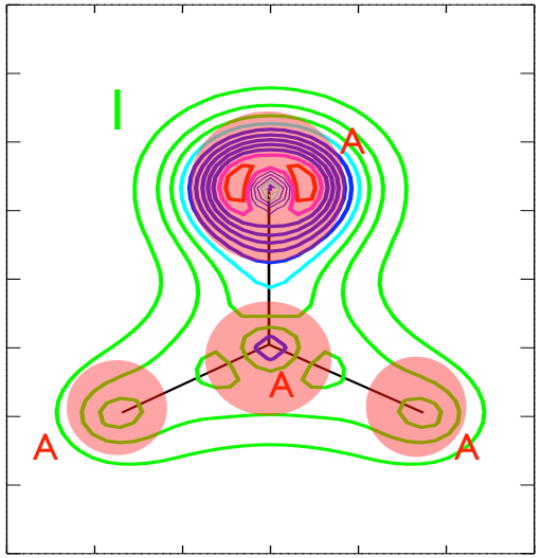
Nodes of ARCHER	45	48	64	96
Original Code	1427	1176	1371	1278
Modified Algorithm	1312	1057	1241	1168
Improvement	8.8%	11.3%	10.5%	9.4%

Table 2: Overall Run Time (seconds).

- Charged cluster of 216 water molecules in 34Å^3 box
- TZV2P MOLOPT basis set
- PBC off
- ~10% speedup

Performance Improvements

- Gaussian and Augmented Plane Waves (GAPW) Method
- Represent core electronic density on spherical grids around each atom
- Avoids frozen-core approximation
- Extra computation not present in GPW:
  - Compute the ‘hard’ density around each atom - `calculate_rho_atom_coeff()`
  - Compute updates to the KS matrix elements for each GAPW atom pair - `update_ks_atom()`
- Not OpenMP parallelised



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Performance Improvements

Version	Processes	Threads	Run Time
Original Code	24	1	273.17
Original Code	6	4	171.25
Implement OpenMP in `update_ks_atom`	6	4	172.30
Implement OpenMP in `calc_rho_atom_coeff`	6	4	73.77
Use hash table in OpenMP in `update_ks_atom`	6	4	61.63
Improve efficiency of OpenMP use & automatic arrays in `calc_rho_atom_coeff`	6	4	47.27

Table 3: Times (seconds) as work on `update_ks_atom` and `calculate_rho_atom_coefficient` progressed

- 32 water molecules in a periodic box
- TZV2P basis set
- GAPW default settings
- 3.6x speedup for whole code

Performance Improvements

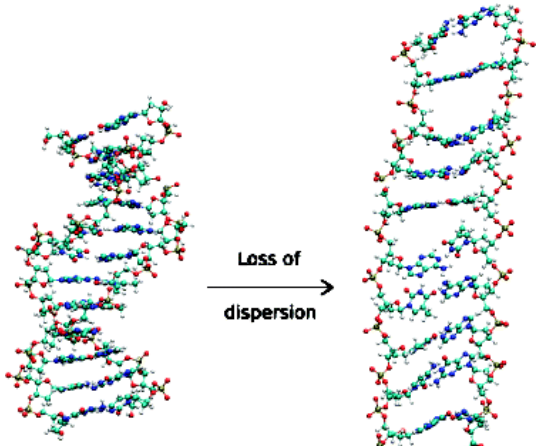
- Dispersion-corrected functionals
  - Important for a wide range of systems:
    - molecular, MOFs, surfaces…
  - Pair-potential type (Grimme D2, D3)
  - Non-local type (vdW-DF, rVV10 …)

- Small but measurable overhead

```
vdW_energy()
get_potential()
calculate_dispersion_pairpot()
calculate_dispersion_nonloc()
```

- Not OpenMP parallelised

Recent overview of vDW corrections in CP2K: https://www.cp2k.org/_media/events:2016_summer_school:cp2k-uk-summer-school-sanliang-ling.pdf



experimental crystal structure

after MD simulation without dispersion terr

$$V(r) = \frac{q_i q_j}{4\pi\varepsilon_0 r_{ij}} + 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\right.\right.$$

Hobza et al. J. Am. Chem. Soc., 130, 16055 (2008)

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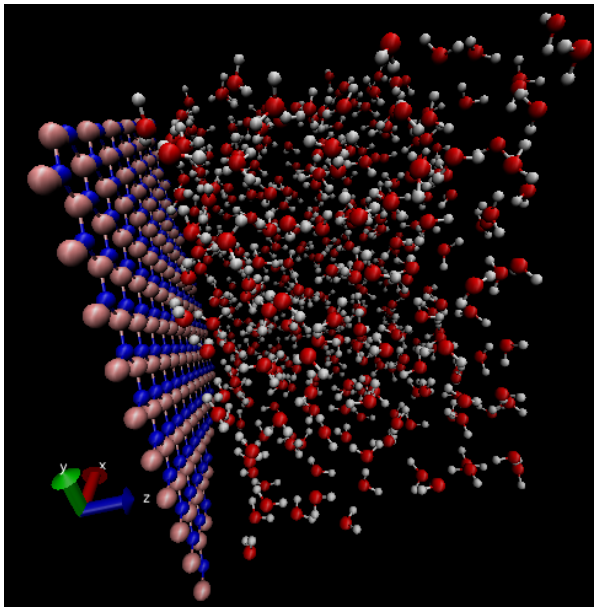
Performance Improvements

	Original		Final	Speedup
	Pure MPI	360 MPI 2 OMP	360 MPI 2 OMP	
Entire Program	414.7	425.4	402.4	1.057×
`calculate_dispersion_nonloc`	9.27	9.61	5.49	1.750×
`vdW_energy`	18.20	34.34	21.61	1.589×
`get_potential`	6.09	6.12	2.63	2.327×

Table 1: Run times (seconds) for routines involved in WP3.

- Water / BN interface
- 400 H_2O, 120 BN
- 1440 atoms, 26x25x40Å cell
- DZVP MOLOPT basis
- optB88-vDW functional (Libxc)
- ~5% speedup



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