CP2K-UK: Supporting Advances in Atomistic Simulation Capability
I. Bethune*1, G. Gibb1, L. Kantorovich2, M. Watkins3, S. Chulkov3 and B. Slater4

1EPCC, The University of Edinburgh 2 King’s College London 3 University of Lincoln 4 University College London

Project Overview
CP2K [1] is a freely available open-source program for atomistic simulation, best known for its implementation of the QUICKSTEP Gaussian and Plane Waves (GPW) linear-scaling Density Functional Theory (DFT) method [2]. However, CP2K provides a much wider range of capabilities, including classical pair-potentials and force-fields, QM/MM, semi-empirical Hamiltonians, hybrid density functionals and double-hybrid methods including Møller-Plesset 2nd order perturbation theory (MP2) [3], the Random Phase Approximation (RPA) [4], and GW [5]. Built at top of these Hamiltonians are an extensive set of simulation tools including Molecular Dynamics, Monte Carlo, Nudged Elastic Band, path integrals and free energy methods. Thus CP2K appeals to a wide range of users including Computational Chemists, Materials Scientists, Solid State Physicists and Biochemists. Usage of CP2K is growing, to the point where it is now the second most heavily used code on ARCHER, the UK national HPC service.

Support for Users
Networking: Our series of annual user group meetings have proved to be very popular. These include a mixture of talks from key CP2K developers, shorter talks focused on how to use particular functionality in the code, and three minute lightning talks, highlighting the breadth of research supported by CP2K. Slides from previous meetings are available at www.cp2k.org/docs#workshops

Training: The CP2K-UK project offers both through classroom-based training events, and bespoke training days with individual research groups. A group we visited in 2014 subsequently received a substantial award of CPU time through the ARCHER Resource Allocation Panel (RAP), leading to a publication [6].

Performance: CP2K offers excellent performance and scalability, but choosing the optimal set of parameters and parallelisation settings is not always straightforward. We carried out systematic benchmarking using a range of different calculation types on several HPC machines [7]. These results are available on the CP2K website along with scripts for plotting performance graphs (www.cp2k.org/performace), and we encourage users to contribute benchmarks from their own machines.

Tools: We have developed a visual web-based tool for editing CP2K input files, complete with tooltip help, and automatic input validation. Within a few minutes, it is possible to create a new input from scratch, or start with an existing one and modify it, then download the resulting file and run it using CP2K. The Input Editor supports all CP2K releases since 2.5 and is available for use at: cp2kInputEditor.epcc.ac.uk

Support for Developers
We have worked on improving CP2K source code quality to make it easier for new developers to understand and contribute to the project. The entire CP2K code-base now contains automatically-generated ‘doxygen’ documentation, which can be browsed online at doxygen.cp2k.org. In addition, we have extended the CP2K automated regression test environment to cover use of the Intel Fortran compiler and MKL library, IBM’s XL Fortran, OpenMPI, and macOS, and now have reliable results on these platforms.

We have also implemented several new methods in CP2K which will be of wide benefit to the community:

- Longevin Dynamics with arbitrary thermal regions [8]
- Filter matrix diagonalisation [9], a scheme were a minimal basis set is constructed dynamically during the SCF procedure which spans a new subspace, guaranteed to contain the minimum energy configuration.
- Fast linear response TDDFT with hybrid density functionals using the Auxiliary Density Matrix Method [10]
- DeltaSCF excited state calculations using the Maximum Overlap Method [11]
- Initialisation of MD velocities based on vibrational analysis to avoid long equilibration runs [12]

Get Involved
CP2K-UK’s primary purpose is to benefit the CP2K community – so if you are already using CP2K, have specific features or methods you want to find out more about, or are just starting to investigate CP2K, then we would like to hear from you! Here are some of the ways you can get involved:

- Want to get started with CP2K? Contact us to arrange a hands-on introduction to CP2K at your institution, with specific focus on your application areas.
- The CP2K website (www.cp2k.org) is now a wiki and anyone can contribute. Please make improvements, contribute tutorials based on your own experience, or ask if you think information is missing.
- Have an idea for a new feature or tool that you’d like to see implemented in CP2K? Talk to us about software development funding opportunities and training.
- If you are applying for a research grant involving CP2K, or wish to use CP2K on ARCHER, contact us to see how we can support your application – letters of support are available!
- To stay in the loop about upcoming CP2K events, we maintain a notification-only email list. Contact us to subscribe.

For any of the above, or if you have other questions about the CP2K-UK project, please email i.bethune@epcc.ed.ac.uk