ARCHER eCSE Final Report

eCSE Number:	02-09
eCSE Title:	Optimising vdW simulations with CASTEP code
Date of Submission:	01/06/2015
PI and Co-Is	M Probert, P Hasnip, K Refson, A Reilly
Technical staff member(s)	Matthew Hodgson
Author of this document	Matthew Hodgson
Project start date	01/09/2014
Project completion date	30/04/2015
Total number of funded project months	7 (+1 month no-cost extension)

1 Publishable Report

1.1 *Achievements and Impact*

Performance improvements

CASTEP had a simple sum method for calculating the van der Waals (vdW) interaction. In this project, this was replaced by a modified Ewald scheme for calculating the vdW energy, force, stress and first order differential of the force for phonon calculations. This has produced a speed up of around a factor of five (in a benchmark water calculation) over the previous implementation in serial. We have also parallelized this code using MPI, whereas the previous code was only serial. Hence for large calculations on ARCHER the code is now many times faster due to the combination of both of these improvements.

A straightforward implementation of the Ewald scheme for 1/r^6 potentials for the calculation was proven to be inadequate, so we developed a modification to the vdW interaction at short ranges. This modification removes the pathologies and allows efficient calculations in even the most extreme cases – these are now over ten times faster in serial and many times faster on ARCHER.

Additional functionality

The code can now calculate the derivative of the vdW contribution to the force with respect to ionic positions which is required for the calculation of phonons and may also be of use in some optimisation routines. Hence it is now possible to perform phonon calculations for materials including vdW interactions.

We have also developed an alternative form of the damping function which is used at short ranges (which can be used in conjunction with any of the existing vdW schemes), which gives rise to a more physically reasonable force, and stress contribution from ions which are closer together than the van der Waals radius. This causes a small rigid shift in the energies of such systems but this is not important for calculating physical observables.

Enabled Science

The new vdW interaction routines can now be used to calculate the contribution to the phonon spectra from the van der Waals interaction.

In addition, the improvements in performance and scaling enable calculations that previously were infeasible. One such test case is the molecular dynamics study of high pressure methane (which arises in the study of gas giant planets).

Impact

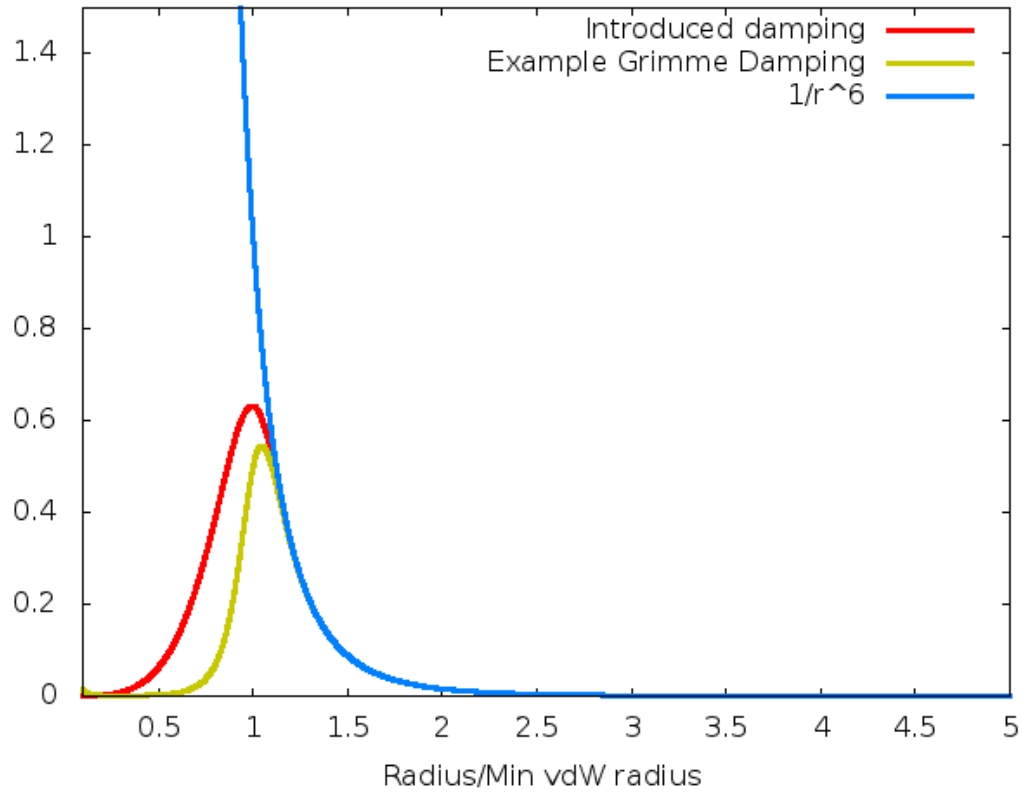
The inclusion of vdW interactions will no longer be a significant bottleneck in any calculation, enabling a large range of calculations to be carried out that previously were infeasible. Such interactions are crucial in the study of many molecular crystals, layered materials, etc – all of which are of great interest. In addition this project has brought to light shortcomings in the current treatment of the van der Waals interaction at short ranges which will be further explored.

1.2 *Publishable summary*

The project was to improve the performance of the van der Waals interactions as implemented in CASTEP. The existing code used various "Semi-Empirical Dispersion Correction" (SEDC) schemes, but performed poorly for a small number of pathological cases, and was not parallel. Hence there were situations where CASTEP run time on machines like ARCHER were dominated by calculating these interactions.

In the SEDC schemes, the vdW interaction is included via a pairwise term between atoms $i$and j of the form $E_{vdW} = C_{ij} f_{damp}(r)/r^6$, with the form of the interaction strength (C_{ij}) and the damping function $f_{damp}(r)$varying between schemes.

We implemented a modified Ewald summation scheme to calculate the SEDC energy, force (and its differential) and stress. This was calculated for a modified potential which damped out the short range contribution, with corrections to the "true" short range behaviour added separately (see figure). This investigation uncovered some unusual behaviour in the SEDC schemes at short distances that could explain the strange impact of van der Waals on materials that has been observed before, where it would not be expected to be a significant contribution.



1.3 *Summary of the software*

CASTEP is a general purpose code for the quantum simulation of properties of materials. It has been developed in the UK for many years, and is widely used within both academia and industry. It is freely available to all UK academics subject to a simple licence agreement. It has been used as part of the acceptance test suite on successive national supercomputers, including ARCHER, and is available on ARCHER as a system binary to all registered users. CASTEP is also available for source-code download from CCPForge (http://ww.ccpforge.cse.rl.ac.uk) for all registered users. CASTEP is also available commercially for industrial and non-UK-academic users from BIOVIA (http://accelrys.com/products/materials-studio).

In this project, the previous implementation of the vdW interaction via the different SEDC schemes has now been replaced by an Ewald summation method. The new routines are now fully integrated into the main CASTEP source, and are currently subject to beta-testing within the core CASTEP developers group. The routines will be part of the next CASTEP release (due Q4 2015) and hence will be in the next ARCHER system binary and future commercial releases. The changes will not be obvious to a casual user as the user interface has not been affected, but all SEDC users will benefit from the speed boost, and affected ARCHER users will see a dramatic effect due to the parallelization.