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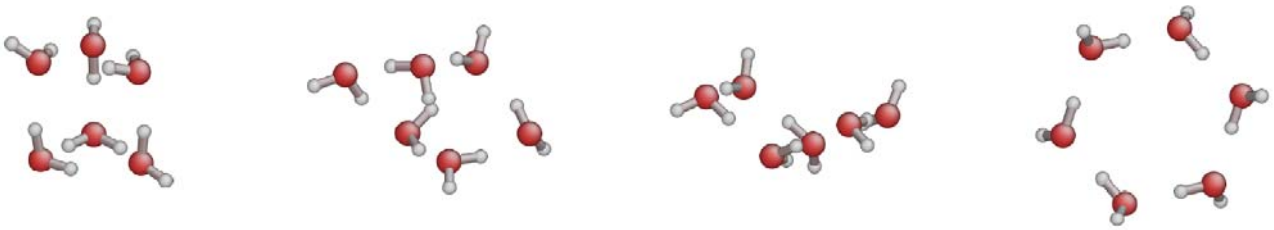
Gaussian Approximation Potential (GAP)

Fast and accurate atomistic modelling technique



Typical isomers of the small cluster of 6 water molecules, the basic representative building block of bulk water, which is often thought of as a 3-dimensional network of hydrogen bonded molecules.

Gaussian Approximation Potential (GAP) is a novel atomistic modelling technique using a patented method to massively accelerate the generation of large sets of atomic configurations and energies, compared to existing Quantum Mechanical modelling tools. GAP may be used either in "corrective mode" (running alongside existing DFT code such as CASTEP or VASP), or in "standalone mode". The corrective mode is fully developed and ready for commercialisation and the standalone mode is still under development.

Applications:

- **Corrective-mode GAP** is ideal for small molecules that are weakly bound such as water, either pure or with solutes. It is also suitable for biological molecules. For details of systems already modelled see overleaf.
- **Standalone-mode GAP** has been used for strongly bound materials, eg non-molecular materials such as metals and silicon, but can also be used more broadly.

Lead inventor:

Dr Gabor Csanyi is a Reader in Engineering at the University of Cambridge, and winner of the Friedrich Wilhelm Bessel Research Award (Alexander von Humboldt Foundation)

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Background

GAP takes established mathematical methods from computer science and applies them to molecular modelling. GAP uses a Bayesian probabilistic algorithm to interpolate a database that is generated a priori using quantum mechanics. Therefore, instead of continually running computationally expensive quantum mechanical models, the user need only build the database once.

Benefits

In Standalone mode, GAP allows the accuracy of quantum mechanical modellers (eg CASTEP, ONETEP, VASP, MOLPRO) to be achieved at the speed of quicker but less accurate modellers (eg TIP3P, AMBER, CHARMM).

In Corrective mode, GAP simply eliminates errors inherent in DFT models, running at the same speed as the uncorrected models.

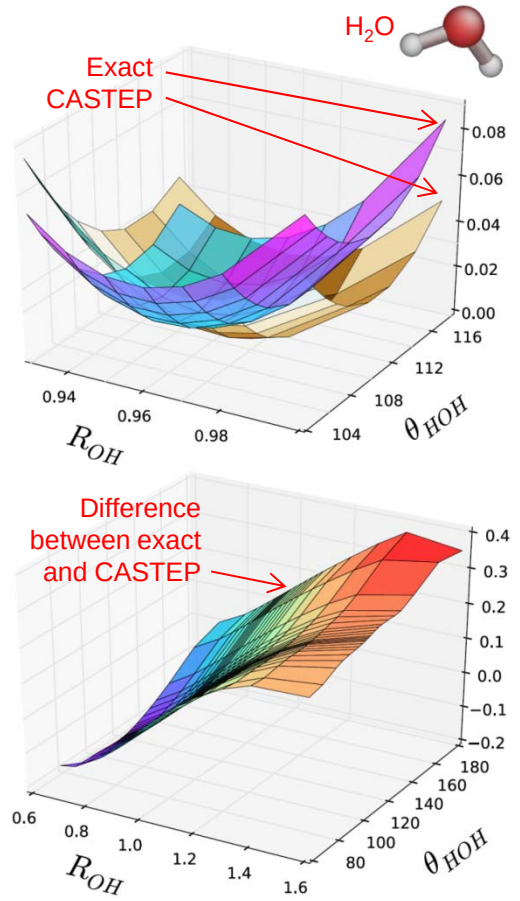
Technology

GAP comprises three software modules and a growing body of data (GAP Models):

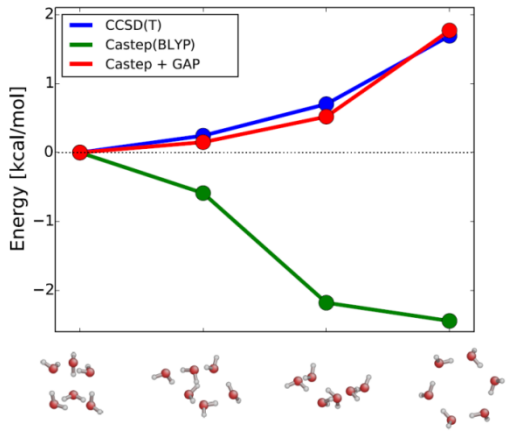
- **Software modules**
  - The GAP prediction algorithm
  - GAP "training code", used to develop GAP Models for each system
  - QUIP, a software wrapper via which GAP integrates with existing DFT and MD codes
- **GAP Models (Corrective-mode)**
  - Water & ice – fully developed & published
    - Eliminates 95% of CASTEP errors
  - Nitrate ion in water – developed and needs benchmarking
  - Gas hydrates (methane, CO_2) – developed and needs benchmarking
  - Solvated ions (eg Li) – under development
  - Other solutes in water – development planned
- **GAP Models (Standalone-mode)**
  - Tungsten – developed & published in 2014
  - Silicon – under development

Applications

GAP is applicable to a broad range of markets, but current development is targeted towards gas hydrates and water with small solutes which are important in the energy and oil & gas sectors.



The images above show discrepancies from CASTEP to empirical data for bond lengths and angles for water. The graph below shows the near elimination of these discrepancies for four different configurations of six water molecules when the GAP correction is applied to CASTEP.



Commercialisation

Cambridge Enterprise is now seeking a partner with whom to collaborate on developing and implementing a commercialisation strategy for GAP.

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