

## Next Generation Simulation Techniques

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In less than twenty years, the plane wave pseudopotential technique has progressed from modelling two atoms of silicon to modelling many hundreds of atoms of any species. However, this technique is still far away, both in terms of accessible lengthscale and more importantly accessible timescale, from being able to address many scientific challenges. In this talk I shall discuss two new techniques which confront these lengthscale and timescale challenges. They are a linear scaling first principles total energy technique, which will be described in greater detail in the talk by Dr. Skylaris, and a hybrid modelling scheme, developed in collaboration with Dr. Sandro De Vita. The linear scaling code provides the same accuracy as the plane wave pseudopotential technique but can be applied to systems containing many thousands of atoms, with the prospect of tens of thousands of atoms in the near future. The hybrid modelling scheme provides the same accuracy as a full quantum mechanical calculation but allows simulations to be performed on systems containing hundreds of thousands of atoms or more for very long simulation times.