INTERATOMIC POTENTIALS FROM FIRST PRINCIPLES (APPROXIMATION AND PARAMETERISATION OF EQUIVARIANT SET FUNCTIONS)

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ABSTRACT

High fidelity atomistic simulation requires computationally expensive quantum chemistry models that make simulating complex material phenomena or large molecules computationally intractable. Much of computational science therefore involves multi-scale modelling or coarse-graining such models to obtain cheaper surrogates such as mean field models, tight-binding models or interatomic potentials. For example, if a simulation task is concerned solely with mechanics of atomic nuclei (treated as classical particles) then the electronic degrees of freedom could be integrated out entirely.

Traditionally such coarse-grained models for the atomic interaction laws were developed via a combination of asymptotic analysis and ad hoc modelling which has resulted in models with poor accuracy and transferrability. The integration of "machine learning" has resulted in a paradigm shift in this field, replacing ad hoc modelling with systematic approximation. The interaction laws that we aim to coarse-grain can be naturally described as *equivariant set functions*: functions defined on atomic configurations (multi-sets) which transform in a specified way under certain group actions that must be exactly preserved.

In this talk I will outline these challenges and explain how such approximation schemes can be constructed in a natural way, leading to the *Atomic Cluster Expansion* (ACE) method. I will sketch out a preliminary end-to-end theory for the ACE method merging ideas from modelling, analysis and numerical analysis to explain at least in principle how rigorous error control can be achieved in each step, both during parameterisation and prediction stages.

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