Novel Interatomic Potentials with Uncertainty Quantification & Applications

MSc/PhD Project Proposal for Mathematics for Real-World Systems CDT

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A. Background. The basic building blocks of materials are their constituent atoms and the bonds between them arising from the arrangement of their associated electrons. The ongoing search for predictive descriptions of materials requires computational models that take into account the atomistic and electronic structure as well as macroscopic information such as stress and strain. The challenge is that standard *ab initio* models achieving the required accuracy are unsuitable due to their high computational cost. Traditionally, this challenge has been addressed with computationally efficient empirical atomistic models whose predictive capabilities are limited.

B. Overall Scope. This project (1) contributes to promising recent developments employing machine-learning (ML) and uncertainty quantification (UQ) methodology to construct computationally efficient interatomic potentials with controlled errors (relative to the training data; e.g. electronic structure models); and (2) explore technological applications of the new methodology. There is a range of possible directions within this project, including

- Analysis and software implementation of moment tensor potentials (MTPs)
- Develop a fast feature kernel based on the MTP ideas, to facilitate ML and UQ
- Analyse the role of temperature (i.e. randomness) in MTP fitting
- Analyse how errors in the MTP propagate into errors in simulation outputs
- Develop a coarse-grained MTP incorporating entropy contributions
- Develop MTPs for specific applications, e.g. crack propagation and dislocation climb

C. MSc and PhD Projects. There is considerable freedom in the choice of direction, but a canonical first step suitable for an MSc project would be to

- Study MTPs [1-2] and interatomic potential methodology [2-5]
- Implement a MTP for a well-studied model system such as bulk silicon within the JuLIP molecular dynamics modelling framework (using the Julia language). The software implementation work will be completed as part of a small research team, and the role within the team can be flexible/discussed.
- Time permitting perform a preliminary analytical or computational study of accuracy of MTPs in an elementary application, such as relaxation of a short-ranged crystal defect.

This will naturally lead to a formulation of a PhD project that may incorporate any of the aspects discussed in §B.

D. Applications. The long-term goal of the project is to develop models which improve our understanding of materials processes. The current generation of interatomic potentials lack reliable error bars, and the ensuing lack of predictive power is a cause of great concern to industry. Options for industrial co-funding and/or partners include the supervisor's industrial links: AWE, TWI, Rolls Royce plus CDT partners JLR, Tata steel and Thalys.

E. References

[1] Shapeev AV, Moment Tensor Potentials: a class of systematically improvable interatomic potentials, Multiscale Model. Simul., 14, 1153-1173 (2016)
[2] Podryabinkin EV and Shapeev AV, Active learning of linear interatomic potentials, arXiv:1611.09346 (2016)
[3] Bartok, AP and Payne, MC and Kondor, R and Csanyi, G Gaussian Approximation Potentials: The Accuracy of Quantum Mechanics, without the Electrons. Phys. Rev. Lett., 104 (2010)
[4] Bartók, AP and Kondor, R and Csányi, G On representing chemical environments. Phys. Rev. B, 87 (2013)
[5] Bartők, AP and Csányi, G Gaussian approximation potentials: A brief tutorial introduction. Int. J. Quant. Chem., 115. pp. 1051-1057 (2015)

[1] The choice of first or second supervisor will depend on whether the project will take a more mathematical/analysis or more computational/modelling direction. Both options are possible.