Mathematics+Physics+Data-Driven Interatomic Potentials

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 contributes to a new trend employing machine-learning (ML) and uncertainty quantification (UQ) methodology to construct computationally efficient interatomic potentials with controlled errors (relative to; e.g. electronic structure models); and explores technological applications of the new methodology. There is a range of possible directions within this project, including

- Analyse existing and develop novel atomic environment descriptors
- Explore the role of temperature (i.e. randomness) in fitting interatomic potentials
- Automated data-base generation by targeted sampling of the ab initio PES
- A project may also develop ML for electronic structure and quantum chemistry models
- Develop bespoke regularisation techniques
- Develop IPs for specific applications, e.g. crack propagation or dislocation climb

Methodology may include: gaussian processes, neural networks, polynomial approximation, UQ, algebraic geometry, high-performance scientific computing, numerical analysis.

C. MSc and PhD Projects. There is considerable freedom in the choice of direction, and an MSc project is best discussed with the supervisors. As an example outline, one might consider

- Develop an atomic environment descriptor from permutation invariant polynomials
- Compare polynomial, GP and ANN regression on some example databases
- Time permitting perform a preliminary analytical or computational study of accuracy of 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] Bartõk, 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.