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Colloquium

Multiscale and data-driven methods for the simulation

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Abstract

I will review recent progress on the development and application of advanced atomistic algorithms to simulate chemomechanical systems where local chemistry and long-range stress are tightly coupled, e.g. at the tip of a propagating crack or the core of a dislocation. I will discuss two general approaches (i): hybrid quantum/classical approaches where bond-breaking is treated at the DFT level embedded within a large-scale classical atomistic model to capture elastic relaxation, including recent applications relevant to dislocation motion in tungsten [1] and fracture in diamond [2]; (ii) the construction of machine learning surrogate models either for electronic structure models [3] or at the interatomic potential level, including recent work carried to massively parallelise the Gaussian approximation potential fitting process [4]. If time permits, I will also discuss the importance of robust uncertainty estimates when using surrogate models, and report some recent efforts in this direction [5].

[1] P. Grigorev, A. M. Goryaeva, M.-C. Marinica, J. R. Kermode, and T. D. Swinburne, Acta Mater. 247 118734 (2023)
[2] J. Brixey, T. Cowie, A. Jardine, J. R. Kermode, In Prep (2023)
[3] L. Zhang et al., npj Comput. Mater. 8 158 (2022)
[4] S. Klawohn, J. R. Kermode and A. P. Bartók, Mach. Learn. Sci. Tech. 4, 015020 (2023)
[5] I. Best, T. J. Sullivan and J. R. Kermode, In Prep (2023)

Bioblurb

James Kermode is Professor of Materials Modelling in the School of Engineering at the University of Warwick, where he directs the Warwick Centre for Predictive Modelling (WCPM) and co-directs the EPSRC Centre for Doctoral Training in Modelling of Heterogeneous Systems (HetSys). I develop multiscale materials modelling algorithms and the software that implements them, with a particular focus on machine learning and data-driven approaches, and on quantifying the uncertainty in the output of electronic structure and atomistic models. He is also active in applying parameter-free modelling techniques to make quantitative predictions of chemomechanical materials failure processes where stress and chemistry are tightly coupled.

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