

MM 28: Invited talk De Vita

Time: Wednesday 9:30–10:00

Location: TC 006

Invited Talk

MM 28.1 Wed 9:30 TC 006

Accurate and fast machine learning n-body force fields

— ALDO GLIELMO¹, CLAUDIO ZENI¹, JAMES KERMODE², and
•ALESSANDRO DE VITA^{1,3} — ¹King's College London, Strand, London WC2R 2LS, UK — ²Warwick Centre for Predictive Modelling, University of Warwick, Coventry CV4 7AL, UK — ³Department of Engineering and Architecture, University of Trieste, I-34127, Trieste, Italy

Modelling phenomena that couple complex local chemistry with higher scales, such as stress corrosion, embrittlement or friction is beyond the reach of first-principles MD techniques. Recent Machine Learning (ML) approaches might achieve the necessary accuracy [1] and, coupled with “on the fly” learning [2] and flexible use of large QM

databases, offer a way to tackle the validation problem. However, ML-based MD simulations are not, as yet, mainstream. Key outstanding issues are how to construct ML-based schemes that are (i) verifiably more accurate than the available parametrised force fields (FFs) while being (ii) as efficient for incorporating prior knowledge on the target systems and (iii) as fast for predicting MD forces. I will review these problems, and discuss how they might be solved by Gaussian Process regression techniques using n-body covariant force kernels whose predicted forces can be suitably “remapped” to give new, fully efficient n-body non-parametric machine-learning force fields (“M-FFs”)[3-4].
[1] F.Bianchini et al., Mod. Sim. Mat. Sci. Eng. 24, 045012 (2016)
[2] Z.Li et al, Phys. Rev. Lett., 114, 096405 (2015) [3] A.Glielmo et al., Phys. Rev. B 95, 214302 (2017) [4] A.Glielmo et al., in prep.