Warwick Centre for Predictive Modelling Seminar Series

Applying machine learning to quantum mechanics

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Thursday, 11th Jun, 4 p.m.
R0.12, Ramphal Building, Ground Floor

Abstract: The talk will report on our efforts in the last few years in attempting to speed up quantum mechanical atomic scale materials modelling by using modern machine learning methods. The task is simple in principle: the forces on atoms that are needed to run a simulation is the gradient field of a high dimensional potential energy function that is smooth almost everywhere, and the calculation of these forces takes all the time in practice and gives rise to poor scaling (O(N^3) - O(N^7) depending on the method, N is number of particles). Making a practical scheme that will have a real impact turns out to be far from trivial. Along the way, we have learned a lot about Bayesian modelling, regularisation of regression and representation theory.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars