Machine Learning Accelerators for Quantum Transport

Luke Keenan[1], Stefano Sanvito[2], Urvesh Patil[3], Declan Nell[4]
[1]Trinity College Dublin, College Green, Dublin, Ireland
[2]Trinity College Dublin, College Green, Dublin, Ireland
[3]Trinity College Dublin, College Green, Dublin, Ireland
[4]Trinity College Dublin, College Green, Dublin, Ireland

lukeenan@tcd.ie

Electron transport is a key phenomenon in modern technology, particularly in transistor logic operations and magnetic data storage. The current state of the art for simulating transport in nanoscaled devices is density functional theory combined with the nonequilibrium green's function formalism, as implemented in the SMEAGOL code [1]. Unfortunately, the computational overheads of this method are typically a hundred times larger than standard DFT and limit the scale and complexity of the problem one can tackle. We aim to train and implement a lightweight machine-learning-driven cluster expansion [2] to predict the non-equilibrium charge density of a gold metallic point contact and its transport properties. This uses a grid- centred structural representation based on Jacobi and Legendre polynomials combined with linear regression to infer the results of large systems, having sampled a limited number of structures [3]. The full workflow is illustrated in Fig 1. This model can be implemented in molecular dynamics simulations, opening new possibilities for studying electron transport at finite temperature.

References

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Figures

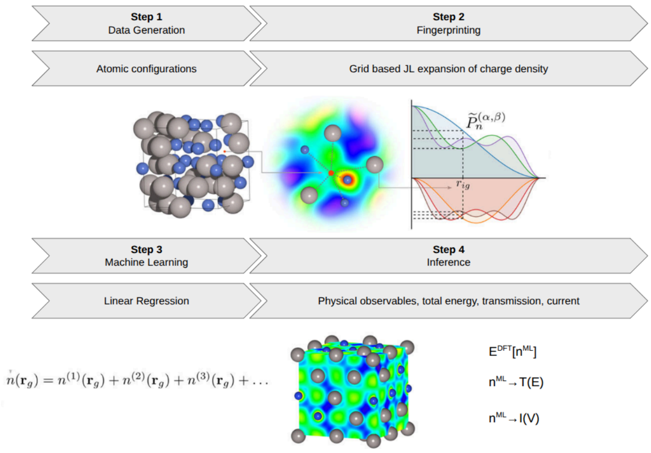

Figure 1. Workflow to construct the linear model that predicts converged DFT ground state density and associated observables. Firstly (step 1), the atomic distribution is mapped over a cartesian grid, where each point is associated with a local atomic environment encoded by the Jacobi - Legendre expansion (step 2). This expansion is used to construct a linear model (step 3) that is trained to predict the charge density of the grid point. The charge density is computed over the entire grid (step 4) followed by the calculation of total energy, forces, transport properties or any density dependent observables.