

Rapid and Rigorous Learning Simulation Methodology with High Accuracy for Electronic and Optical Superlattices

Martin Veresko, Yu Liu, Daqing Hou and Ming-Cheng Cheng*

Department of Electrical and Computer Engineering
Clarkson University, Potsdam, NY 13699-5720, USA

*mcheng@Clarkson.edu

Abstract. A rigorous physics-informed learning methodology is proposed for predictions of wave solutions and band structures in electronic and optical superlattice structures. The methodology is enabled by proper orthogonal decomposition (POD) and Galerkin projection of the wave equation. The approach solves the wave eigenvalue problem in POD space constituted by a finite set of basis functions (or POD modes). The POD ensures that the generated modes are optimized and tailored to the parametric variations of the system. Galerkin projection however enforces physical principles in the methodology to further enhance the accuracy and efficiency of the developed model. It has been demonstrated that the POD-Galerkin methodology offers an approach with a reduction in degrees of freedom by 4 orders of magnitude, compared to direct numerical simulation (DNS). A computing speedup near 15,000 times over DNS can be achieved with high accuracy for either of the superlattice structures if only the band structure is calculated without the wave solution. If both wave function solution and band structure are needed, a 2-order reduction in computational time can be achieved with a relative least square error (LSE) near 1%. When the training is incomplete or the desired eigenstates are slightly beyond the training bounds, an accurate prediction with an LSE near 1%-2% still can be reached if more POD modes are included. This reveals its remarkable learning ability to reach correct solutions with the guidance of physical principles provided by Galerkin projection.

Keywords: Proper orthogonal decomposition, model order reduction, Galerkin projection, wave eigenvalue problems.