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Simulating long-term diffusive heat and mass transport phenomena in nanoscale systems

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Zoom

In this presentation, I will introduce a formulation and computational package to simulate long-term diffusive mass transport in systems with atomic scale resolution. The implemented framework is based on a non-equilibrium statistical thermo-chemo-mechanical formulation of atomic systems where effective transport rates are computed using a kinematic diffusion law. Our implementation is built as an add-on to the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) code, it is compatible with other LAMMPS' functionalities, and shows a good parallel scalability and efficiency. In applications involving diffusive mass transport, this framework is able to simulate problems of technological interest for exceedingly large time scales using an atomistic description, which are not reachable with the *state-of-the-art* molecular dynamics techniques. Several examples, involving complex diffusive behavior in materials, are investigated with the framework. We found good qualitative and quantitative comparison with known theories and models, with Monte Carlo methods, as well as with experimental results. Thus, our implementation can be used as a tool to understand diffusive behavior in materials where experimental characterization is difficult to perform.

Bio:

Dr. Mauricio Ponga has been an Assistant Professor in Mechanical Engineering at UBC and joined as a faculty member in 2016. Ponga is also affiliated with the UBC Institutes of Applied Mathematics and Computing, Information and Cognitive Systems (ICICS), and the Advanced Materials and Process Engineering Laboratory at UBC. Ponga is an expert in computational mechanics, modelling and simulation, with a specific focus on multiscale and multiphysics phenomena in materials at the nanoscale. Ponga's research group develops novel modelling techniques to analyze coupled problems in nanoscale systems. These techniques include large-scale ab-initio methodologies, coarse-grained molecular dynamics, coupling phonons and electrons in molecular dynamics simulations, mechanics of polymer brushes, etc. These techniques extend the realm of atomistic simulations and represent the state-of-the-art modelling tools for materials at the nanoscale. Ponga has been awarded several allocations in HPC facilities, including the prestigious and competitive U.S. Department of Energy ALCC allocation with more than 20 million CPU hours to the use of large-scale ab-initio simulations, and about 3 million CPU hours from Compute Canada. Ponga's research has been supported by NSERC (Alliance, DG, Engage), the New Frontiers in Research Funds, and the IDEaS program by the Department of National Defence and many other industrial partners in Canada.

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