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Dynamic coupling of a finite element solver to large-scale atomistic simulations

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ABSTRACT

We propose a method for efficiently coupling the finite element method with atomistic simulations, while using molecular dynamics or kinetic Monte Carlo techniques. Our method can dynamically build an optimized unstructured mesh that follows the geometry defined by atomistic data. On this mesh, different multiphysics problems can be solved to obtain distributions of physical quantities of interest, which can be fed back to the atomistic system. The simulation flow is optimized to maximize computational efficiency while maintaining good accuracy. This is achieved by providing the modules for a) optimization of the density of the generated mesh according to requirements of a specific geometry and b) efficient extension of the finite element domain without a need to extend the atomistic one. Our method is organized as an open-source C++ code. In the current implementation, an efficient Laplace equation solver for calculating the electric field distribution near a rough atomistic surface demonstrates the capability of the suggested approach.

1. Introduction

Achieving atomistic spatial and temporal resolution is still challenging for experimental physics and, in many cases, numerical simulations based on well-motivated physical models are the only tools which can provide interesting insight on the atomic scale. However, due to an unavoidable trade-off between computational efficiency and desired accuracy, often seemingly promising computational models turn out to be impractical.

One way to achieve high computational efficiency and numerical accuracy is to combine continuous-space calculations with atomistic simulations like classical molecular dynamics (MD) or kinetic Monte Carlo (KMC). Some such approaches [1–4] have shown promising results when simulating the elastoplastic evolution of nanostructures. Others [5–9], being especially relevant to the present work, have used such a technique to study the effects of electric field around nanostructured materials.

When a strong electric field is applied on the surface of a metal, it induces surface charge and polarization, and under certain circumstances, it triggers field emission (FE) currents with consequent electromigration effects [10]. Thus, the high electric field may significantly affect the evolution of the system and under certain conditions might cause major surface

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deformations [11]. For that reason, atomistic simulations that take into account the effects of electrostatic field have a wide range of applications in atom probe tomography (APT) [12], nanoelectronics [13] and space technology [14]. Moreover, atomistic modeling is a valuable tool in the investigation of vacuum arcing phenomena (vacuum breakdowns), as the fundamental mechanisms that trigger a breakdown are not entirely clear yet. The breakdown studies are relevant to the development of new-generation linear colliders like CLIC in CERN [15], vacuum interrupters [16], free electron lasers [17] and fusion devices [18].

Simulating electronic processes on material surfaces requires an accurately calculated spatial distribution of the electric field. The common method for calculating the field around any geometry is to build a mesh around the system of interest and solve the Laplace or Poisson equation on it. The solver is usually based on the finite difference method (FDM) [9,19], finite element method (FEM) [7] or their modifications [6]. Many authors [8,20] calculate the electric field around nanostructures without building any mesh around it. Although such mesh-free methods might be more flexible and efficient under certain conditions, they are limited in practical applications as they incorporate only the calculation of electric field.

The mesh for solving the differential equations can be either static (it does not change during the evolution of the underlying atomistic geometry) or dynamic (the mesh is adjusted with the movement of the atoms). Both can be either structured or unstructured. The main advantage of a structured mesh is its implementation simplicity, while the unstructured one provides higher tolerance to the underlying geometry. Although the generation of an unstructured dynamic mesh requires significant computational effort, it has considerable advantages over the alternatives. Since it is reconstructed at every simulation step, its shape will accurately follow the underlying geometry with the optimal density in each region. This ensures high robustness against changes in the crystallographic structure of the material, good scalability and maximum accuracy for a given computational cost.

Effects of electric field, thus far, have been introduced in atomistic simulations based on a structured or unstructured static mesh approaches. The mesh that is generated in those works either lacks accuracy in following the underlying geometry [7] or is unnecessarily dense [6], making the total computational cost unfeasible to be performed iteratively. Also, previous works are rather not universal as they typically focus on a specific type of differential equations.

The present work is the continuation of our previous attempt to include the electronic effects in atomistic simulations by solving the Laplace equation on a structured static mesh using FDM [5]. This method enabled us to investigate the behavior of Cu surface under high electric field when small-scale surface features are present [21–26]. However, the high computational cost and inflexible mesh limited the earlier simulations to specific crystal structures and orientations, few nm scale and very short times. To cope with the forthcoming challenges of large scale dynamic simulations, we generalized the method by combining the dynamic mesh approach with the FEM. In this way, we provide a framework for solving multiple differential equations in vacuum and material domains, to achieve enhanced computational efficiency, scalability and tolerance with respect to the crystallographic structure of studied materials. The framework also allows us to use the results in iterative atomistic simulations like MD and KMC.

To a large extent the current work is motivated by vacuum arc studies. For that reason, we demonstrate the potential of our approach by calculating electric fields around metal nanotips which are considered to cause vacuum arcing [27,28]. The value of the electric field that is found near the surface of the metal nanotip can be used to calculate electrostatic forces acting on atoms by the field as well as Coulomb forces due to partial charging of surface atoms as demonstrated in [5] and [29]. Those forces, in turn, perturb the atomic movement [5]. Similar conditions, i.e. presence of high electric fields around metal nanotips also appear in FE [30–32] and APT [6,8,12] studies, where our approach of combining atomistic and continuum calculations can be very useful.

2. Methodology

2.1. Overview

The main objective of the current project is to provide a tool for calculating the effects of electric field on atomistic systems for up to 10^7 atoms with a reasonable computational effort. For that purpose, we provide an open-source C++ code that contains the modules which enable to:

- import atomistic coordinates of a nanostructure from the atomistic simulation;
- dynamically generate an unstructured mesh around the imported structure;
- solve the differential equations of interest on the mesh;
- return the solution to the atomistic simulation.

By using FEM for solving the differential equations, we can optimize the mesh density in various parts of the simulation domain. In regions of high interest, where the solution changes rapidly, the mesh can be made denser and in regions with small solution gradient and lower interest the mesh could be coarser. However, generating a mesh with appropriate density is rather obligatory as performing the calculation on a poorly optimized mesh is impractical in terms of computational cost. In our simulations, we are mostly interested in the processes that take place on the surface of the material. For that reason, the mesh we generate to follow the surface geometry is dense near the surface, becoming gradually coarser away from it. However, to meet the needs of a wider audience, such an optimization scheme can be overridden by the user.