# The Atomic Limit of Finite Elements in the Simulation of Micro-Resonators

Robert E. Rudd

University of Oxford, Department of Materials
Parks Road, Oxford OX1 3PH England
robert.rudd@materials.ox.ac.uk
http://users.ox.ac.uk/~rudd/GrandChallenge

## ABSTRACT

We describe developments in the coupling of length scales methodology which allows the simulation of the dynamic and temperature dependent behavior of sub-micron Micro-Electro-Mechanical Systems (MEMS). This novel technique accurately models the behavior of the mechanical components of MEMS down to the atomic scale, by combining the power of an atomistic simulation with the efficiency of finite elements. The codes have been written using scalable algorithms suitable for parallel supercomputers. In this paper we discuss the general issues involved in this type of multiscale simulation, with a particular emphasis on the behavior of finite elements when the mesh spacing is refined to the atomic scale and methods for generating such a mesh. We also describe some results from simulations of the vibrational behavior of sub-micron silicon and quartz oscillators.

***Keywords***: MEMS, silicon resonators, coupling of length scales, finite elements, molecular dynamics

## 1 Modeling Sub-micron MEMS

The growing interest in mechanical devices less than a micron in size for use in Micro-Electro-Mechanical Systems (MEMS) has posed a new challenge for the development of reliable design and analysis tools. In this Article we describe one solution: the use of multiscale models to provide a robust description of MEMS in the sub-micron regime. These models significantly extend the range of validity of conventional modeling techniques through the inclusion of atomistic physics in parts of the simulation where it is required. Nearly all modeling and simulation of MEMS relies on finite element analysis, which is a discretization of the continuum theories that form the foundation of engineering analysis. Continuum equations such as Hooke's Law of Elastic Theory and the Navier-Stokes Equations of Fluid Dynamics offer extremely powerful descriptions of systems including MEMS, provided they are large enough. At small scales, the basic assumption of theories of continuous media is patently false: *at the Angstrom scale materials are not continuous media, but are composed of discrete atoms.*

The challenge for modeling sub-micron MEMS is that the the smallest of the cells used in the finite element mesh need to be at this atomic scale, and the model is forced treat this atomic limit correctly in order to produce meaningful results. On the other hand, in even the smallest MEMS devices that can be envisioned, there are regions whose behavior is governed by continuum physics. Mechanical members are attached to a substrate and fluids flow from a reservoir. These regions contain a macroscopic number of atoms. It would be inefficient, and perhaps prohibitively computer-intensive, to simulate each atom in these regions: conventional finite elements is clearly the correct tool here.

Neither conventional finite elements nor pure atomistics alone would suffice to describe a sub-micron MEMS device in its entirety. The tool that is required must combine the accuracy of atomistics with the efficiency of finite elements, each used in the regions where it is needed. This is the philosophy behind concurrent multiscale simulation and the coupling of length scales. [1], [2] Standard finite element models are modified to give the correct atomic limit and a smooth crossover from the continuum to the atomic scale.

In this Article we focus on the solid mechanical aspects of the MEMS devices, although many of the issues we discuss could equally well apply to the fluid mechanics or the interactions with external fields. The main device we model is a flexural mode microresonator. It is a long thin bar that has been etched from a single crystal and remains attached at both ends. An example made by the Roukes group is shown in Fig. 1 [3] and it is simulated as shown in Fig. 2. The bar resonates like a violin string. The resonant frequency increases as the device size decreases; currently, the prototypes made by the Roukes group have a resonant frequency on the order of a gigahertz. They are made from single crystals, which leads to drastically reduced dissipation and a greatly enhanced quality factor, Q. There are many applications for high quality gigahertz resonators, including frequency standards and filters for communications. [4] Similar devices have been proposed for novel scientific uses such as producing squeezed states. [5]

This Article describes the multiscale methodology and how it allows the finite element mesh spacing to be refined to the atomic scale. We describe how the methodology works in general terms, with references to the literature [1], [2] for specific details.

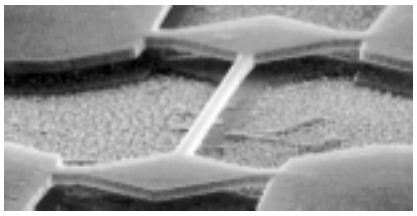

Figure 1: Prototypical microresonator. Courtesy of Prof. M. Roukes, Cal Tech. (See Ref. [3])

## 2 Why Conventional Finite Element Analysis Fails in the Atomic Limit

We have argued that finite element models are unreliable in the atomic limit, but the exact way in which they fail can vary greatly from system to system. In particular, both the scale at which errors arise and the form that the pathologies take depend on the situation. We have found that deviations from the bulk predictions often arise as surface and edge terms in physical quantities such as the resonant frequency of the oscillator. These terms scale as the surface area to volume ratio and the edge length to volume ratio, respectively, which are irrelevant to large devices. They can dominate the behavior of small devices, however, and multiscale simulation is one way to ensure that such effects are captured even if they are not anticipated.

Another problem with finite elements at small scales is the potential importance of non-linear effects, even when negligible at larger scales. The use of transferable atomistic models in the atomic limit guarantees the correct non-linear behavior without the need for additional parameters. This in turn allows the direct simulation of atomic scale processes. For instance, it is possible to directly observe mechanisms contributing to dissipation, device failure, plastic deformations, impurity diffusion, and so on. The multiscale simulation opens new horizons for device modeling. Of course, often the result of these simulations is a new set of constitutive relations that govern the device performance for a particular range of sizes and geometries, and these constitutive relations may be used in conventional finite element models.

## 3 Multiscale Methodology

The methodology that implements the coupling of length scales involves a hybridization of finite elements (FE) with molecular dynamics (MD), an atomistic model. MD is used in those regions that demand atomic-scale accuracy; a conventional FE model is used elsewhere. In concurrent multiscale modeling, both MD and FE run simultaneously, passing information back and forth across an interface, often called the handshaking region. The details of this coupling have been given elsewhere, [1], [2] so we will only briefly review the concepts here.

Figure 2: The silicon microresonator as simulated. The long, thin bar in the middle of the device is only attached to the substrate at the ends, so that it is free to oscillate. The oscillations are out of the plane of the device. Different bar sizes have been simulated with the same substrate geometry.

We have developed two techniques for constructing the MD/FE interface. The first technique, Coarse-Grained Molecular Dynamics (CGMD), [6] produces a truly seamless interface by directly integrating out short wavelength degrees of freedom in order to derive a generalized FE model. The second technique uses only conventional finite elements, and a minimal FE/MD coupling. [2] We will focus on the latter method in this Article. The FE mesh is refined to the atomic scale, with mesh nodes placed at the equilibrium positions of the MD atoms. The FE mesh supports a displacement field, which is constrained at the FE/MD interface to agree with the atomic displacement of the corresponding MD atom. At the interface, both the nodal displacement and the MD atom see the same force: the average of the MD and FE forces. Since the forces are the same, and the initial FE displacement is chosen to equal the initial MD displacement at the interface, the two representations of the displacement are equal at all subsequent times. This achieves a coupling between the MD and FE models.

Due to space limitations in this Article, we cannot go into the details about the FE and MD models. The FE model we have used is based on linear elastic theory, so the parameters are the elastic constants and the density. The MD models use 3-body empirical potentials that have been validated extensively for silicon (the Stillinger-Weber potential) [7] and quartz (the LSU potential) [8]. Also, note that while the coupling of length scales methodology has been extended to include quantum mechanical forces in order to model crack propagation [9], the MEMS simulations to date have only used the FE/MD coupling.

## 4 Mesh Generation

The problem of mesh generation takes on new dimensions for concurrent multiscale simulations (See Fig. 3). In regions of large mesh size, the usual rules governing mesh generation apply. [10] The size of the mesh spacing is set by the scale of changes or fluctuations in the fields. In particular, in type-$h$ adaptive refinement the

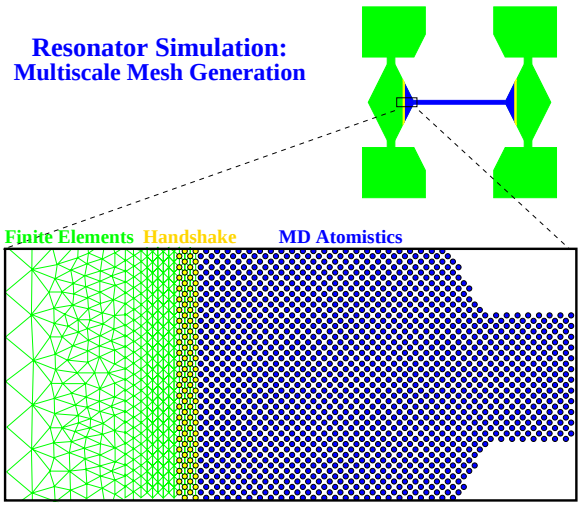


Figure 3: Example of a 2D finite element mesh that is refined down to the atomic scale. Note that molecular dynamics is used in the central part of the device and finite elements in the periphery according to the scales set by the geometry. Generally, 3D FE has been used.

decision to add or remove nodes is based on some estimate of the error as a function of cell size. [10] Another requirement is that the aspect ratio of the cells not vary too much from unity. High aspect ratio cells can lead to numerical pathologies. [10]

In regions where the mesh spacing is at the atomic scale, different considerations apply. The nodes of the mesh should be co-located with, and in one-to-one correspondence to, the atomic lattice positions, so that mass is localized to the nodes. In the case of many metals, the closest-packed lattice leads to a typical FE mesh, but for semiconductors the meshes are quite different. For example, silicon has a diamond-cubic atomic lattice. The atoms are tetrahedrally coordinated, so that the nearest neighbors of each atom are arranged symmetrically about that atom at the apices of a tetrahedron. The diamond-cubic lattice is much more open than the closest-packed lattices, leading to a rather atypical FE mesh.

The challenge for mesh generation is that the mesh should interpolate smoothly between the true atomic lattice in the MD region and the closest-packed meshes that are appropriate in the periphery. Too abrupt a crossover leads to unphysical behavior, such as elastic wave resonances at the interface. [6] Since the need to match onto an atomic lattice first arose with the advent of multiscale simulation, the appropriate mesh generation tool did not exist, and it was necessary for us to construct an algorithm. We have developed a technique that is able to generate large multiscale meshes in 2D and 3D relatively quickly. In particular, the time to generate the mesh scales with the number of mesh points: it is order-N.

The idea for the mesh generation algorithm is based on energy minimization. In the atomic limit, the forces between the nodes/atoms are governed by an empirical interatomic potential, as described above:

$$V = \sum_{A<B} V_2(\vec{r}_A, \vec{r}_B) + \sum_{A<B,C} V_3(\vec{r}_A, \vec{r}_B, \vec{r}_C) \qquad (1)$$

where $V_2$ and $V_3$ are 2-body and 3-body terms, respectively. The total potential energy is minimized when the atoms are arrayed in the correct lattice with the correct lattice spacing. In the case of silicon, the atoms prefer the diamond-cubic lattice because of $V_3$. The 3-body term depends on the angle formed by triplets of neighboring atoms: in particular, it is minimized when this angle is 109°, the central angle for a tetrahedron. The 2-body terms are roughly of the Lennard-Jones form, with a strong short-range repulsion, a weak long-range attraction and consequently a minimum at the correct interatomic spacing. It is the 2-body terms that set the lattice constant. Together the 2- and 3-body terms produce the physical diamond-cubic lattice when the total potential energy is minimized.

The goal is to generate a mesh with a given spacing $\rho(\vec{r})$, where $\rho = 1$ for atomic spacing in the MD region and $\rho > 1$ in the FE region. To achieve this, a mesh-generating potential is used in which the 2-body terms are rescaled:

$$V_{\rm mesh}(\vec{r}_A; \rho) = \sum_{A<B} V_2(\vec{r}_A/\rho, \vec{r}_B/\rho) + \sum_{A<B,C} V_3(\vec{r}_A, \vec{r}_B, \vec{r}_C) \qquad (2)$$

This gives the correct atomic lattice when $\rho = 1$, and a closest-packed lattice optimal for finite elements when $\rho \gg 1$, and there is a smooth crossover in between.

In general, minimization of $V_{\rm mesh}$ is an order-$N^2$ problem. This kind of problem would typically be solved using a Krylov subspace technique such as conjugate gradient minimization, [11] modulo possibile pathologies due to trapping of the minimization trajectory in a local minimum of the potential. In general, defects arise during the minimization process that are akin to the grain boundaries, dislocations and vacancies of solid state physics. The topological defects can be 'annealed out' after a number of steps of order $N^2$, the amount of time necessary to cross the system. Fortunately, it is not essential to achieve the absolute minimum of the potential. As long as the defects do not violate the requirements, well-shaped cells of the desired sizes and a smooth crossover to the atomic lattice, the mesh will produce a well-behaved finite element model. Since the defects are essentially irrelevant to the FE performance, we have chosen to forego annealing, in favor of very rapid mesh generation.

The algorithm we have designed is an order-N advancing front technique based on minimization of the

scaled interatomic potential. The mesh is generated as follows. First the atomic mesh is generated in regions where $\rho = 1$. Next $V_{\rm mesh}$ is computed on a regular grid with spacing of about 1/3 the interatomic spacing. Since the potential is short-ranged, the energy is zero for most of the grid points. Verlet lists are used for efficient computation of the energy. Next the first node for the finite element region is placed at the grid point with the lowest energy, and it is moved from there to the local minimum of the potential using the conjugate gradient technique. The total energy is updated with the contribution of the new node. Then nodes are added one-by-one, in the same way until there are no grid points left with negative energies. At this point the entire mesh in the finite element region is relaxed with a few steps of conjugate gradient minimization. This is an order-N process since each node is placed at a local minimum a fixed number of times. Thus, a high quality multiscale mesh is produced very rapidly.

## 5 Results of MEMS Simulations

We have described the results of our initial simulations of MEMS resonators elsewhere. [2], [1] One important result was that the Young's modulus of quartz resonators deviates from its bulk value for devices 0.1 $\mu$m long and less. [12] The deviation is proportional to the surface area-to-volume ratio, and it causes a reduction in the Young's modulus (which in turn determines the resonant frequency of the oscillator). The deviation is due to atomistic processes at the surface of the resonator, something that could not have been predicted from a continuum or finite element model.

In our other work, we have carried out direct simulations of the oscillations of quartz and silicon resonators of various sizes but with an aspect ratio of 25:2:1. In a typical run, the resonator has been allowed to come to thermal equilibrium at the temperature of interest. Then it has been deflected into one of its normal modes, and the resulting oscillations have been observed. At cryogenic temperatures, very pure oscillatory modes result: there is negligible transfer of energy out of the primary mode during the time simulated. This has been the case for all of the system sizes we have simulated (0.02 - 0.2 $\mu$m long). This predicts very high Q values at low temperatures.

At room temperature, the situation is different (see Fig. 4). For small systems, the oscillations are seen to degenerate markedly during the course of the simulation. Spectral analysis has revealed that energy is transferred from the mode that is initially excited into the neighboring harmonics, a reflection of an anharmonic coupling of the modes. This effect is dependent on the system size, in that smaller systems show greater dissipation and hence smaller Q values.

Currently, the focus of our DoD HPC Grand Challenge project is the study of dissipation in sub-micron resonators as a function of device size, composition and geometry, as well as temperature. As mentioned above, the multiscale technique not only permits the determination of the Q-value of the device, but it allows the precise dissipation mechanisms to be identified. This work will be presented elsewhere. [13]

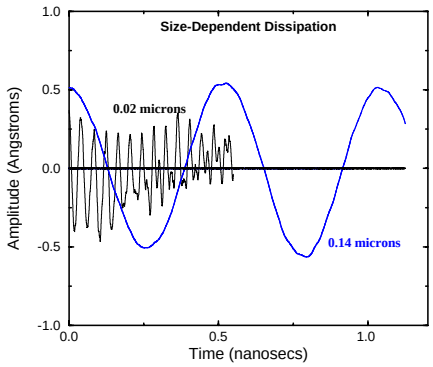


Figure 4: Comparison of the oscillations of resonators of the same aspect ratio but different lengths, both at room temperature. Note the increased dissipation in the smaller resonator.

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