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Mechanical Computation, Redux?

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Abstract

Nanoscale mechanical devices offer the prospect of signal processing, computation, and sensing – at microwave frequencies, sub-nanosecond time scales, and with unprecedented sensitivity and consumption of extremely small amounts of power. In this brief paper I will review the current state-of-the art of nanoelectromechanical systems (NEMS) – with respect to both the underlying fundamental science, and realized (or *realizable*) applications. The paper concludes with my speculations regarding the future role of nanomechanics in computation, in the context of the rich and rather surprising history of (macroscale) mechanically-based logic.

Introduction

One can argue that our contemporary, collective imagination has been tyrannized by things electronic: by default we equate "device" to *electronic* device (*i.e.* transistor), and "system" to digital electronic computer. But it is only since the middle of the twentieth century that such a mindset has become entrenched; the intuition of previous generations was firmly rooted in the domain of *mechanical* objects.

More than one hundred and sixty years ago Charles Babbage conceived of an "analytic engine" – a bona fide *programmable* computer based upon mechanical operations. It was replete with a central processor (*"the mill"*) and a separate mechanical memory (*"the store"*). He envisaged algorithmic programming input by punched cards, with similar technology for the machine's numerical output. Among its design features were logical operations that included looped instructions and conditional branching. Surprisingly, Babbage's profoundly visionary foresights of the 1830's had arguably no impact upon the development of modern digital computer, even though they predated those of von Neumann by more than a century (1). In fact it was not until the late twentieth century that a team led by Doron Swade at the Science Museum in London confirmed and vindicated Babbage's prescience. In 1991, the team successfully completed and operated Babbage's *"Difference Engine No. 2"* – translating some twenty engineering drawings, constituting Babbage's complete blueprints for its construction, into computing machinery that had never been realized in his lifetime (2). The contrast between, on one hand, Babbage's incredible foresight and, on the other, his negligible influence upon the modern history of digital computation should give us significant pause for reflection, especially today as we attempt to transition nanoscience into real technology. We shall return to such considerations at the conclusion of this paper.

Possible Forms of Mechanical Computation

Mechanical computation can be carried out in two distinct forms. First, as envisaged by Babbage and others, linear or angular displacement of mechanical parts can form the basis for multistate logic, with logic "state" being physically manifested as a spatial configuration of the functional parts themselves, with state changes orchestrated by parts displacement. Second, computation could be based upon acoustic "waves" – *i.e.* the vibrational modes of mechanical elements. This dynamical form of mechanical computation need not be limited to the domain of reversible computation; non-linear response of dissipative mechanical elements can provide the basis for non-reversible logic operations (3,4).

In actuality, these two methods of operation are not as distinct as might first be imagined. Even for linear displacements of mechanical elements, dynamical response is crucial to determining the maximal speed of unit operations – the resonant modes of the mechanical elements themselves and their respective damping factors determine the time scale on which a logic element can be "switched" between mechanical states. We shall return to this point.

Nanoelectromechanical Systems (NEMS)

A. Overview: Important Attributes for Mechanical "Logic"

Nanoelectromechanical systems, or NEMS, are MEMS scaled to submicron dimensions (5,6). In this size regime, it is possible to attain extremely high fundamental frequencies while simultaneously preserving very high mechanical responsivity (small force constants). This powerful combination of attributes translates directly into fast mechanical response times, operability at ultralow power, and the ability to induce usable nonlinearity with quite modest control forces. These are briefly detailed below.

Employing these attributes involves the substantial challenge of obtaining optimal actuation and displacement transduction; one finds that mainstays from MEMS (for example, capacitive- and optically-based detection) do *not* scale well down to extreme sub-micron scale dimensions. Fortunately, there are a host of

Table 1: Fundamental Frequency *vs.* Geometry for *SiC*, [Si], and (GaAs) Mechanical Resonators

Boundary Conditions	**Resonator Dimensions** ($L \times w \times t$, *in* μm)			
	100 × 3 × 0.1	*10 × 0.2 × 0.1*	*1 × 0.05 × 0.05*	*0.1 × 0.01 × 0.01*
Both Ends Clamped or Free	*120 KHz* [77] (42)	*12 MHz* [7.7] (4.2)	*590 MHz* [380] (205)	*12 GHz* [7.7] (4.2)
Both Ends Pinned	*53 KHz* [34] (18)	*5.3 MHz* [3.4] (1.8)	*260 MHz* [170] (92)	*5.3 GHz* [3.4] (1.8)
Cantilever	*19 KHz* [12] (6.5)	*1.9 MHz* [1.2] (0.65)	*93 MHz* [60] (32)	*1.9 GHz* [1.2] (0.65)

other physical processes that can be employed for actuation and transduction, and several of these have proven to be extremely robust for the task over the past few years (7).

B. Frequency and Response Time

Table 1 displays attainable frequencies for the fundamental flexural modes of thin beams, for dimensions spanning from the domain from MEMS (leftmost entries) to deep within NEMS. The mode shapes, and hence the force constants and resulting frequencies, depend upon the way the beams are clamped; Table 1 lists the results for the simplest, representative boundary conditions along three separate rows. Although nanostructures in this size domain have been achievable for more than a decade, microwave-frequency NEMS (>1GHz) have only been realized recently (8). This reflects the aforementioned difficulty of displacement transduction, which requires extreme sub-nanometer scale resolution with large bandwidth. The last column represents dimensions now routinely attainable with advanced electron beam lithography. Even smaller sizes than this have become feasible with bottom up assembly (9,10); clearly the ultimate limits are reached only at the molecular scale. Nanodevices in this molecular regime will have resonant frequencies in the range of THz, characteristic of molecular vibrations.

Each entry is in three parts, corresponding to structures made from silicon carbide, silicon, and gallium arsenide. These materials have been of particular interest to my group given their congruence with conventional semiconductor processes. Accordingly, they are among the “standards” within MEMS. These materials are available with extremely high purity, as monocrystalline layers in epitaxially grown heterostructures. This latter aspect yields dimensional control in the “vertical” (out of plane) dimension at the monolayer level. This is nicely compatible with the lateral dimensional precision of electron beam lithography that approaches the atomic scale. The numbers in the table should be considered loosely as “typical”; they represent rough averages for the commonly used crystallographic orientations.

One might ask at what size scale does continuum mechanics break down and corrections from atomistic behavior emerge. Molecular dynamics simulations for ideal structures appear to indicate that this becomes manifested only at the truly molecular scale, of order tens of lattice constants in cross section (11). Hence, for most initial work in NEMS, it would appear that continuum approximation will be adequate.

C. Operating Power Level

Applications of NEMS resonators will typically involve use of a specific mode. As mentioned, however, even displacement-based mechanical logic will involve modal analysis. A rough understanding of the minimum operating power levels using this mode can be obtained by dividing the thermal energy, $k_B T$, by the characteristic time scale for energy exchange between the mode, at frequency ω_0, and its surroundings (i.e. “the environment”). The time scale is set, roughly, by the “ring-up” or “ring-down” time of the resonator, $\sim Q/\omega_0$. A simple estimate for the minimum power is then given by the ratio,

$$P_{\min} \sim k_B T\, \omega_0 / Q \,. \tag{1}$$

This represents the signal power that must be fed to the system to drive it to an amplitude equal to the thermal fluctuations.

This minimum power is remarkably small for NEMS. For device dimensions accessible today via electron beam lithography, the characteristic level is of order ten attowatts (10^{-17} W). Even if we multiply this upward by a factor of a million, to achieve robust signal-to-noise ratios, and then further envision a million such devices acting in concert to realize some sort of future NEMS-based mechanical computer — the total system power levels still are only of order 1 μW. This is six orders of magnitude smaller than power dissipation in current systems of similar complexity based upon digital devices that work solely in the electrical domain. However this is a bit too optimistic an estimate, at least one inconsistent with achieving logic transition times of order $1/\omega_0$. If we critically damp the devices to achieve such transition times, the Q-factor decreases by four-five orders, increasing the overall system power dissipation evaluated above from the μW level to the 10’s of mW scale. Yet this is still quite respectable.

D. Nonlinearity

The onset of nonlinearity – crucial for many classes of switching applications and for parametric processes – occurs for smaller applied force (hence lower input power) in large aspect ratio structures. In fact, for very large aspect ratio doubly-clamped structures we have recently shown that the linear dynamic range, bounded by the thermomechanical noise floor and the onset of nonlinearity, can vanish – meaning that nanotube resonators are intrinsically nonlinear elements (12) !

The aforementioned example stems from the Duffing instability; for doubly-clamped structures a tension term in the elastic restoring force emerges for modest displacements which provide a nonlinear complement to the predominantly linear “body” forces of beam flexure. We have recently employed this to realize efficient frequency-tuning of NEMS resonators. The Euler instability is a second mechanical nonlinearity that provides opportunity for all-mechanical parametric gain. A high frequency, high gain mechanical amplifier has been recently demonstrated (13). Such concepts could prove important for acoustic logic.

Mechanical Computation: Future Projections

A. Hindsight is 20/20

In his attempts to build computing machines, Babbage faced significant issues given both the lack of standardization of and the reproducibility of manufacture in his times. In his day, screw threads from different machine shops would not match, so a single contractor had to be engaged to build an entire system. The industrial era of interchangeable parts would not arrive until the latter half of the nineteenth century (14). Babbage’s need for high levels of precision and uniformity was exacerbated by his choice of decimal (10-state) logic; a choice of binary logic would have relaxed the switching margins required for system operation. This came back to haunt the team realizing Babbage’s difference engine, even though they benefited from modern-day parts reproducibility.

Production of mechanical systems has evolved from what could be called the “craftsman” era when, for example, individuals produced amazingly intricate clockwork – even though no two shop’s threads were alike, to an era of reproducible and standardized, precision *manufacturing*. The latter enabled interchangeable mass-produced parts. Initially the impact was to enable one-of-a-kind, complex mechanical systems – but these systems still required final parts tweaking (filing, filling, finishing, fitting) to render the system operational. Ultimately, however, with attainment of sufficiently precise tolerances in manufacturing, production *en masse* of modularly-assembled systems became possible. This is perhaps best epitomized by modern automobiles, which achieve astounding metrics in cost-to-complexity, reliability, and mass-production.

For MEMS, and even more so for NEMS, one could argue that we are still in the craftsman era. Individual inventors routinely demonstrate the promise and potential of a new technology, but the era of precise tolerances – especially in nanoscale parts finishes (surfaces) – is not yet upon us. Hence the prospect of assembling architecture of mechanical logic, sufficiently complex so as to be competitive, would seem distant. In this context, a metric suggested by a 2001 JASON panel studying nanobiotechnology, led by S. Block and P. Alivasatos is particularly relevant (15). They defined “negentropy” as $S \sim -\ln$ (error rate, precision, purity, etc.), and point out that Mother Nature’s molecularly precise nanomachines achieve S ~21-24 (specifically, in DNA replication with error correction).

What level of negentropy is likely to be necessary for building a bona fide nanomechanical computer? The Babbage difference engine was built using a negentropy that I estimate to be of order $S \sim 7$ (few mil tolerances on few inch small parts). This was barely enough, since in 1991, as I’ve mentioned, in the final stages, lots of tweaking of parts by hand was involved before *Difference Engine No. 2* became operational. Top-down microfabrication perhaps attains $S \sim 9$ (tenth micron tolerances on mm-scale parts), but this deteriorates rapidly as one scales down in size to top-down *nano*fabrication, $S \sim 1$ to 3. Perhaps the final answer lies in Feynman’s original vision of nanotechnology (16): the ultimate level of precision is attained when constituent parts are placed with accuracy at the atomic scale. In this case relevant values of S are probably set by thermodynamics (or quantum limits), and hence probably best couched in terms of the ratio of atomic vibrations to the size of the structure. But building complex, atomically-assembled mechanical computers is not likely to happen in the next few years. Only in the past year, for example, have the first high frequency nanowire- and nanotube-based mechanical resonators been realized (9,10).

B. Monoliths or Modular Systems?

One-of-a-kind systems suffer from the shortcoming that they are devilishly difficult to debug. The Science Museum team, in the final stages before unveiling their *Difference Engine No. 2*, actually had to *saw* the system apart to replace a part that was found to be out-of-tolerance subsequent to the system’s assembly (1). Despite his overall prescience, Babbage had not designed to allow modular assembly of the whole.

Modularity seems key to building complex systems. But in the case of nanomechanical elements how shall we interconnect the modules? Perhaps information exchange between sub-systems (*e.g.* mechanical logic gates) should best be mediated purely in the mechanical domain. But any realistic form of purely mechanical computation would have to be formulated upon ultra-low dissipation (i.e. nearly frictionless) mechanical interconnects capable of transmitting the output of one gate to others. Such technology has yet to be identified (17). Ideally, there should be the possibility of “gain” in such a interconnection – at least in the sense that the problem of fan-out can be surmounted. For displacement-based mechanical logic this is possible using external energy reservoirs (the weight of levitated parts, or elastic energy of springs), continually recharged by external sources. For dynamical mechanical (acoustic) logic, this is possible using nonlinearities in mechanical response to create parametric mechanical gain, which has been robustly demonstrated (13).

One is tempted to posit that an electromechanical logic gate, perhaps something akin to the electromechanical shuttle (18), might be the ideal "module". But building an architecture based upon such elements involves electrical interconnects. With this conversion back to the electrical domain, our putative "mechanical" computer would now suffer from the bugaboo that plagues many, if not most, proposals for modern nanoscale electronic logic – *interconnects*. It is extremely hard to make a low power computer when you have to sequentially charge and discharge vast lengths of interconnects at high speeds with voltages that overcome thermal fluctuations with sufficient large margins so as to permit computational accuracy.

C. Ultimate Limits and Cross-Domain "Fusion"

The ultimate limits of NEMS are at the molecular or atomic scale – and there the frequencies and time scales are set by the vibrational properties of molecules. The first hint of the future era of *molecular mechanical systems* is in the buckyball resonators realized by Park, McEuen, and collaborators in 2001 (19). In fact, one could argue that molecular electronics and NEMS are actually converging toward the same end goal, at least in terms of future electronics and information processing systems. Both explicitly rely upon mechanical conformations/configurations to derive their functionality, *i.e.* to achieve device "states" upon which logic can be created.

Mother Nature, the premier architect at the molecular scale, uses a full palette of functional domains to achieve her mysteries. By this I mean, for example, that ion channels in cell membranes function by ion transport (ionics), molecular conformation (mechanics), and chemical recognition (biochemistry). We should take heed; future nanotechnology will clearly involve a fusion of many such "domains". To restrict ourselves to any one domain, *e.g.* electronic, is likely to preclude the full spectrum of innovation possible from nanoscience. Mother Nature may not have produced any paradigms for fast logic at the level of individual "devices" (neurons), but what is (at present) *unfathomable* computational efficiency emerges from her mastery of complexity.

D. Evolution or Revolution?

It is probably not possible to realize a workable fusion between existing electronics (*i.e.* CMOS) and nanomechanical devices. This seems true looking at the disparity between the location of the operating dynamic range of NEMS (attowatts to picowatts) and that of CMOS. Evolutionary approaches to merge these two technologies may not be profitable. In fact, this seems to be a truism for much of molecular electronics at large; the full benefits of nanotechnology may require shifting away from the existing, well-understood paradigms of silicon electronics technology that we've invested in so heavily over the past five decades. I know this prospect will not be initially welcomed with open arms; it is one that will be forced upon us through necessity – that is, Moore's Law.

To look for ways to get there from here is probably like barking up the wrong tree. New science presents itself to us at the nanoscale; perhaps optimal focus would be upon creating new functional paradigms from the possibilities that emerge in this domain.

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