Ratchet Computing—The Heat Bath as Computational Resource

Srinandan Dasmahapatra[1], Jörn Werner[2], and Klaus-Peter Zauner[1]
[1]School of Electronics and Computer Science and
[2] School of Biological Sciences
University of Southampton, SO17 1BJ, United Kingdom
{sd,kpz}@ecs.soton.ac.uk, J.M.Werner@soton.ac.uk

All life forms rely on information processing to maintain their highly organised state. Macromolecules are key components of biological information processing—they enable modes of computation fundamentally different from conventional computing. Macromolecules are immersed in a complex, thermal environment providing a spectrum of fluctuations. Rather than suppressing noise biomacromolecules appear to exploit it. The modulation of potentials and the concomitant tuning of transition probabilities traps favourable fluctuations to yield useful functionality. Molecular motors are a prominent example. Arguably this mode of operation underlies many phenomena observed in nature's macromolecular machinery, ranging from catalysis to protein folding. We speculate that subtle trapping of random fluctuations also plays a crucial role in molecular information processing.

Computers, being part of the physical universe, operate within the constraints provided by the laws of physics as we know them; they need to be shielded from entropy production and heat dissipation for them to extract useful work from their energy sources. Biological systems, too, operate within the same set of constraints, yet their spontaneous ordered states and the precision of their genetic information transfer at nano-scales is maintained in an environment where thermal motion is a prominent feature [1]. Biological macromolecules seem to be able to press thermal noise to the services of cells and organisms.

This ability to funnel random fluctuations into a preferred direction is most easily illustrated with molecular motors. The basic idea of their operation can be traced to Feynman's version of a Maxwell Demon implemented as ratchet and pawl [2]. The presence of a ratchet introduces an essential asymmetry into the system. It would appear that this asymmetry could prevent motion in one direction, while allowing the integration of momentum from molecular collisions, effectively rectifying thermal motion. Such a

hypothetical device can't work in practice; at thermal equilibrium the fluctuations in the ratchet mechanism would nullify any rectification. The principle of eliciting directed motion from random fluctuations does work, however, if the potential function of the system is suitably modulated. When molecules experience an asymmetry repeated along some generalised co-ordinate, but in a time-dependent, non-equilibrium fashion, they can generate a drift velocity by averaging over thermal noise [3, 4]. The result is a Brownian molecular motor, i.e. a molecular machine that harvests thermally activated state-transitions to perform useful work. This mechanism has been used to explain the sophisticated operation of the molecular machines that transcribe genetic information [5] and supramolecular machines acting as Brownian motors have been demonstrated with synthetic chemicals [6].

The principle of biased selection from a random pool of possibilities appears to underly not only the evolution of species, but is more broadly applicable in biology, as has been observed by Jerne [7]. It is also applicable to enzymatic catalysis, where substrate binding stabilises conformational states selected from a large set of rapidly traversed conformational fluctuations [8, 9, 10]. Moreover, selection from fluctuations may also be operational at the molecular level of signal transduction. For example, ligand induced biasing of a set of interconverting states that results in a detectable and transmittable molecular change is in agreement with observations on the regulation of protein kinases—some of the most prominent proteins in signal transduction.

Artifical molecular information processing devices (c.f. [11]) face the same noisy environment as their natural counterparts [12]. Selecting the course of computation from random fluctuations by modulation of free-energy landscapes may be a viable approach to tackling thermal noise in a constructive way. We propose to investigate the potential of Brownian ratchets as a mechanism for molecular information processing. In more general terms the trapping of random search can also support the self-organisation of supramolecular architectures [13].

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