Brownian Molecular Computing
(Two steps forward, One step Back)

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Heat dissipation has always been a problem for computers. A modern parallel supercomputer such as IBM’s BlueGene/L, though designed to be energy-efficient, still requires massive amounts of cooling. The fans and air conditioning make so much noise that ear protection is required in the machine room.

Electricity and cooling are also major parts of the cost of commercial server farms.
When Turing, Shannon, von Neumann et al formalized the notions of information and computation, they left out a couple of important ideas:

- **Reversibility**
- **Thermodynamics of Computation**
- **Superposition**
- **Quantum Computation**

(The thermodynamic resources required for computation can be linked to physical states and evolutions, and more mystically, to Wheeler’s “It from Bit”: involvement of information in the creation of physical reality.)
Thermodynamics of Computation

• Landauer’s Principle: each erasure of a bit, or other logical 2:1 mapping of the state of a physical computer, increases the entropy of its environment by $k \log 2$.

• Reversible computers, which by their hardware and programming avoid these logically irreversible operations, can in principle operate with arbitrarily little energy dissipation per step.
Conventional      Efficient 1:1 map      Efficient 2:1 map

Cost $E_B \gg kT$  Cost 0  Cost $kT \ln 2$
Classification of Computers from thermodynamic viewpoint

A. Irreversible (e.g. PC, Mac…)

B. Reversible

1. Ballistic (e.g. Billiard ball model) dynamical trajectory isomorphic to desired computation

2. Brownian (e.g. RNA polymerase) random walk in a low-energy labyrinth in configuration space, isomorphic to desired computation
The chaotic world of Brownian motion, illustrated by a molecular dynamics movie of a synthetic lipid bilayer (middle) in water (left and right)

dilauryl phosphatidyl ethanolamine in water
http://www.pc.chemie.tu-darmstadt.de/research/molcad/movie.shtml
RNA polymerase reaction viewed as a one-dimensional driven random walk

or as thermal diffusion on a washboard potential
Tilting the washboard the other way (e.g. by increasing the PP concentration) makes the driving force negative, resulting in reversible erasure or un-copying of an already synthesized strand of RNA.
Potential Energy Landscape for Brownian Computer

Error probability per step is approx. \( \exp \left[ \frac{(E_0 - E_e)}{kT} \right] \)

Error correction is logically many-to-one, so it has a thermodynamic cost, by Landauer’s principle.

Conversely, and less obviously, a system’s “desire” to make errors is itself a thermodynamic driving force that can be partly harnessed to reduce the cost of correcting the errors.
In the real world, errors occur.
So the RNA copy is not perfect.
But, because the RNA strand separates from the DNA original after leaving the copying enzyme, error transitions have the same driving force as good transitions. Higher activation barrier for error transition.

Copying errors therefore act as *reversible obstructions*, difficult to insert, and equally difficult to remove.

In the presence of errors, even this reversible copying process exhibits a nontrivial tradeoff among, speed, error rate, and dissipation.
Active Proofreading for reliable DNA Replication

Polymerase activity (1) tries to insert correct base, but occasionally (2) makes an error. Exonuclease activity (3) tries to remove errors, but occasionally (4) removes correct bases. When both reactions are driven hard forward the error rate is the product of their individual error rates.
Dissipation mainly in external driving reactions. At high error rate, this pushes process forward even against uphill external driving force.
For any given hardware environment, e.g. CMOS, DNA polymerase, there will be some tradeoff among dissipation, error, and computation rate.

More complicated hardware might reduce the error, and/or increase the amount of computation done per unit energy dissipated.

This tradeoff is largely unexplored, except by engineers.
Error correction is analogous to chemical separations such as distillation. Practical stills have a tradeoff among speed, product purity, and energy dissipation.
But it is wrong to separate hardware from software. Even the simplest hardware can be a fertile ground for self-organization, in effect creating a simulation of more complicated hardware.

But how should complexity be defined? What is it that increases when a self-organizing system organizes itself?

Is dissipation necessary, or sufficient, for this to happen?
Temperature gradient is in the wrong direction for convection. Thus we get static dissipation without any sort of computation, other than an analog solution of the Laplace equation.
Dissipation-error Tradeoff for Computation

50°C  But if the water has impurities

10°C  Turbine civilization can maintain and repair itself, do universal computation.
Ultimate scaling of computation.

Obviously a 3 dimensional computer that produces heat uniformly throughout its volume is not scalable.

A 1- or 2- dimensional computer can dispose of heat by radiation, if it is warmer than 3K.

Conduction won’t work unless a cold reservoir is nearby. Convection is more complicated, involving gravity, hydrodynamics, and equation of state of the coolant fluid.
Fortunately 1 and 2-dimensional fault tolerant universal computers exist:

e.g. cellular automata that correct errors by a self-organized hierarchy of majority voting in larger and larger blocks, even though all local transition probabilities are positive.
(P. Gacs math.PR/0003117)
Self-organization, the spontaneous increase of complexity. A simple dynamics (1 dimensional reversible cellular automaton) can produce a complicated effect from a simple cause.

Small irregularity (green) in initial pattern produces a complex deterministic “wake” spreading out behind it.
Range-2, deterministic, 1-dimensional Ising rule. Future differs from past if exactly two of the four nearest upper and lower neighbors are black and two are white at the present time.
A sufficiently big piece of the wake (red) contains enough evidence to infer the whole structure. A smaller pieces (blue) does not.
In the philosophy of science, the principle of Occam's Razor directs us to choose the most economical hypothesis able to explain a given body of observed phenomena.

Alternative Hypotheses  

Deductive Reasoning

Observed Phenomenon

Most economical hypothesis is preferred, even if the deductive path connecting it to observation is long.
Logically deep objects contain internal evidence of having undergone a long and complicated evolution.
A trivially orderly sequence like $111111\ldots$ is logically shallow because it can be computed rapidly from a short description.

A typical random sequence, produced by coin tossing, is also logically shallow, because it essentially its own shortest description, and is rapidly computable from that. Depth thus differs from Kolmogorov complexity or algorithmic information, defined as the length of the shortest description, which is high for random sequences.
At equilibrium, complexity still persists in 2-time correlations. Two time slices of the equilibrated system contain internal evidence of the intervening dynamics, even though each slice itself is shallow. The inhabitants of this world, being confined to one time slice, can’t see this complexity. (Also they’d be dead.)
In an equilibrium world with local interactions (e.g. a thermal ensemble under a local Hamiltonian) correlations are generically local, mediated through the present.

By contrast, in a non-equilibrium world, local dynamics can generically give rise to long range correlations, mediated not through the present but through a V-shaped path in space-time representing a common history.


CHB on Logical Depth, 2012 see blog http://dabacon.org/pontiff/?p=5912

Reversibility of RNA polymerase: backward operation in presence of excess pyrophosphate

(extra slides)
Connection of thermal disequilibrium with memory stability and self-organization, or stabilization of complex structures:

- Gibbs phase rule: for generic parameter values, a locally interacting classical system, of finite spatial dimensionality and at finite temperature, relaxes to a unique Gibbs state of lowest bulk free energy.

=> no long term memory

=> as \( N, t \to \infty \), complexity (e.g. in the sense of logical depth) remains bounded

- Dissipative exception
- Quantum exception, in 3 or more dimensions.
Classical dissipative systems can systems evade Gibbs phase rule

Phase region is a narrow metastable zone (demarcated on the right by dashed lines), in which large islands of the favored phase grow but small islands shrink. A critical exponent of $3.0 \pm 0.4$ was found for the vertical width of the two-phase region as a function of noise amplitude $(p + q)$ below the critical point. Other runs on one-phase systems with unbiased noise $p = q$ yielded the value $\beta = 0.122 \pm 0.01$ for the exponent describing magnetization as a function of noise amplitude below the critical point.

Besides being irreversible, the NEC model differs from conventional kinetic Ising models in having synchronous updating. However, preliminary runs in

Toom's NEC rule stable against generic symmetry-breaking field in 2d => Gacs-Reif fault tolerant cellular automaton in 3D
Toom Rule Snapshots at different points on phase diagram
Phase Diagram of Classical Ising model in \(d > 1\) dimension. Stores a classical bit reliably when \(T=0,\) or \(h=0\) and \(T<T_c\)

Phase diagrams for local quantum models (Toric code)

- **\(d = 2\)**
  - \(h = 0\)
  - \(T_c\)
  - Degenerate ground state stores a qubit reliably at \(T=0,\) even for nonzero \(h.\) For \(T>0,\) stores a bit reliably only at \(h=0\)

- **\(d = 3\)**
  - \(T_c\)
  - Stores a qubit at \(T=0.\) For \(T>0,\) can store a quantum-encoded classical bit, even when \(h\) is nonzero

- **\(d = 4\)**
  - \(T_c\)
  - Stores a quantum-encoded qubit even at nonzero \(T\) and \(h.\)

(the end)