Selim G. Akl Cristian S. Calude
Michael J. Dinneen Grzegorz Rozenberg
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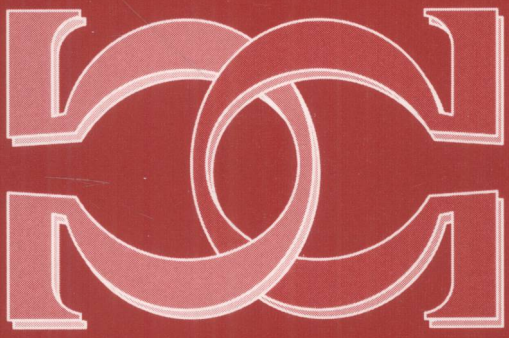
Unconventional Computation

6th International Conference, UC 2007
Kingston, Canada, August 2007
Proceedings



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Preface

The Sixth International Conference on Unconventional Computation, UC 2007, organized under the auspices of the EATCS by the Centre for Discrete Mathematics and Theoretical Computer Science (Auckland, New Zealand) and the School of Computing, Queen's University (Kingston, Ontario, Canada) was held in Kingston during August 13–17, 2007. By coming to Kingston, the International Conference on Unconventional Computation made its debut in the Americas.

The venue for the conference was the Four Points Hotel in downtown Kingston on the shores of Lake Ontario. Kingston was founded in 1673 where Lake Ontario runs into the St. Lawrence River, and served as Canada's first capital. Renowned as the fresh-water capital of North America, Kingston is a major port to cruise the famous Thousand Islands. The 'Limestone City' has developed a thriving artistic and entertainment life and hosts several festivals each year. Other points of interest include Fort Henry, a 19th century British military fortress, as well as 17 museums that showcase everything from woodworking to military and technological advances.

The International Conference on Unconventional Computation (UC) series, `https://www.cs.auckland.ac.nz/CDMTCS/conferences/uc/`, is devoted to all aspects of unconventional computation, theory as well as experiments and applications. Typical, but not exclusive, topics are: natural computing including quantum, cellular, molecular, neural and evolutionary computing; chaos and dynamical system-based computing; and various proposals for computations that go beyond the Turing model.

The first venue of the Unconventional Computation Conference (formerly called Unconventional Models of Computation) was Auckland, New Zealand in 1998; subsequent sites of the conference were Brussels, Belgium in 2000, Kobe, Japan in 2002, Seville, Spain in 2005, and York, UK in 2006.

The titles of volumes of previous UC conferences are the following:

1. C. S. Calude, J. Casti, and M. J. Dinneen (eds.). *Unconventional Models of Computation*, Springer-Verlag, Singapore, 1998.
2. I. Antoniou, C. S. Calude, and M. J. Dinneen (eds.). *Unconventional Models of Computation, UMC'2K: Proceedings of the Second International Conference*, Springer-Verlag, London, 2001.
3. C. S. Calude, M. J. Dinneen, and F. Peper (eds.). *Unconventional Models of Computation: Proceedings of the Third International Conference, UMC 2002*, Lecture Notes in Computer Science no. 2509, Springer-Verlag, Heidelberg, 2002.
4. C. S. Calude, M. J. Dinneen, M. J. Pérez-Jiménez, Gh. Păun, and G. Rozenberg (eds.). *Unconventional Computation: Proceedings of the 4th International Conference, UC 2005*, Lecture Notes in Computer Science no. 3699, Springer, Heidelberg, 2005.

5. C. S. Calude, M. J. Dinneen, Gh. Păun, G. Rozenberg, and S. Stepney (eds.). *Unconventional Computation: Proceedings of the 5th International Conference, UC 2006*, Lecture Notes in Computer Science no. 4135, Springer, Heidelberg, 2006.

The Steering Committee of the International Conference on Unconventional Computation series includes T. Bäck (Leiden, The Netherlands), C. S. Calude (Auckland, New Zealand (Co-chair)), L. K. Grover (Murray Hill, NJ, USA), J. van Leeuwen (Utrecht, The Netherlands), S. Lloyd (Cambridge, MA, USA), Gh. Păun (Seville, Spain and Bucharest, Romania), T. Toffoli (Boston, MA, USA), C. Torras (Barcelona, Spain), G. Rozenberg (Leiden, The Netherlands and Boulder, Colorado, USA (Co-chair)), and A. Salomaa (Turku, Finland).

The four keynote speakers of the conference for 2007 were:

- Michael A. Arbib (U. Southern California, USA): *A Top-Down Approach to Brain-Inspired Computing Architectures*
- Lila Kari (U. Western Ontario, Canada): *Nanocomputing by Self-Assembly*
- Roel Vertegaal (Queen's University, Canada): *Organic User Interfaces (Oui!): Designing Computers in Any Way, Shape or Form*
- Tal Mor (Technion–Israel Institute of Technology): *Algorithmic Cooling: Putting a New Spin on the Identification of Molecules*

In addition, UC 2007 had two workshops, one on Language Theory in Biocomputing organized by Michael Domaratzki (University of Manitoba) and Kai Salomaa (Queen's University), and another on Unconventional Computational Problems, organized by Marius Nagy and Naya Nagy (Queen's University). Moreover, two tutorials were offered on Quantum Information Processing by Gilles Brassard (Université de Montréal) and Wireless Ad Hoc and Sensor Networks by Hossam Hassanein (Queen's University).

The Programme Committee is grateful for the much-appreciated work done by the paper reviewers for the conference. These experts were:

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We extend our thanks to all members of the local Conference Committee, particularly to Selim G. Akl (Chair), Kamrul Islam, Marius Nagy, Yurai Núñez, Kai Salomaa, and Henry Xiao of Queen's University for their invaluable organizational work. We also thank Rhonda Chaytor (St. John's, NL, Canada) for providing additional assistance in preparing the proceedings.

We thank the many local sponsors of the conference.

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- MITACS - Mathematics of Information Technology and Complex Systems
- IEEE, Kingston Section

It is a great pleasure to acknowledge the fine co-operation with the *Lecture Notes in Computer Science* team of Springer for producing this volume in time for the conference.

May 2007

Selim G. Akl
Christian S. Calude
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Invited Papers

Regular Papers

How Neural Computing Can Still Be Unconventional After All These Years

Michael A. Arbib

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Abstract. Attempts to infer a technology from the computing style of the brain have often focused on general learning styles, such as Hebbian learning, supervised learning, and reinforcement learning. The present talk will place such studies in a broader context based on the diversity of structures in the mammalian brain – not only does the cerebral cortex have many regions with their own distinctive characteristics, but their architecture differs drastically from that of basal ganglia, cerebellum, hippocampus, etc. We will discuss all this within a comparative, evolutionary context. The talk will make the case for a brain-inspired computing architecture which complements the bottom-up design of diverse styles of adaptive subsystem with a top-level design which melds a variety of such subsystems to best match the capability of the integrated system to the demands of a specific range of physical or informational environments.

This talk will be a sequel to *Arbib, M.A., 2003*, Towards a neurally-inspired computer architecture, *Natural computing, 2*:1-46, but the exposition will be self-contained.

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Optimal Algorithmic Cooling of Spins

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Abstract. *Algorithmic Cooling (AC) of Spins* is potentially the first near-future application of quantum computing devices. Straightforward quantum algorithms combined with novel entropy manipulations can result in a method to improve the identification of molecules.

We introduce here several new exhaustive cooling algorithms, such as the Tribonacci and k-bonacci algorithms. In particular, we present the "all-bonacci" algorithm, which appears to reach the maximal degree of cooling obtainable by the optimal AC approach.

1 Introduction

Molecules are built from atoms, and the nucleus inside each atom has a property called "spin". The spin can be understood as the orientation of the nucleus, and when put in a magnetic field, certain spins are binary, either up (ZERO) or down (ONE). Several such bits (inside a single molecule) represent a binary string, or a register. A macroscopic number of such registers/molecules can be manipulated in parallel, as is done, for instance, in Magnetic Resonance Imaging (MRI). The purposes of magnetic resonance methods include the identification of molecules (e.g., proteins), material analysis, and imaging, for chemical or biomedical applications. From the perspective of quantum computation, the spectrometric device that typically monitors and manipulates these bits/spins can be considered a simple "quantum computing" device.

Enhancing the sensitivity of such methods is a Holy Grail in the area of Nuclear Magnetic Resonance (NMR). A common approach to this problem, known as "effective cooling", has been to reduce the entropy of spins. A spin with lower entropy is considered "cooler" and provides a better signal when used for identifying molecules. To date, effective cooling methods have been plagued by various limitations and feasibility problems.

"Algorithmic Cooling" [1,2,3] is a novel and unconventional effective-cooling method that vastly reduces spin entropy. AC makes use of "data compression" algorithms (that are run on the spins themselves) in combination with "thermalization". Due to Shannon's entropy bound (source-coding bound [4]), data compression alone is highly limited in its ability to reduce entropy: the total entropy of the spins in a molecule is preserved, and therefore cooling one spin is done at the expense of heating others. Entropy reduction is boosted dramatically

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by taking advantage of the phenomenon of thermalization, the natural return of a spins entropy to its thermal equilibrium value where any information encoded on the spin is erased. Our entropy manipulation steps are designed such that the excess entropy is always placed on pre-selected spins, called "reset bits", which return very quickly to thermal equilibrium. Alternating data compression steps with thermalization of the reset spins thus reduces the total entropy of the spins in the system far beyond Shannon's bound.The AC of short molecules is experimentally feasible in conventional NMR labs; we, for example, recently cooled spins of a three-bit quantum computer beyond Shannon's entropy bound [5].

1.1 Spin-Temperature and NMR Sensitivity

For two-state systems (e.g. binary spins) there is a simple connection between temperature, entropy, and probability. The difference in probability between the two states is called the *polarization bias*. Consider a single spin particle in a constant magnetic field. At equilibrium with a thermal heat-bath the probabilities of this spin to be up or down (i.e., parallel or anti-parallel to the magnetic field) are given by: $p_\uparrow = \frac{1+\varepsilon_0}{2}$, and $p_\downarrow = \frac{1-\varepsilon_0}{2}$. We refer to a spin as a bit, so that $|\uparrow\rangle \equiv |0\rangle$ and $|\downarrow\rangle \equiv |1\rangle$, where $|x\rangle$ represents the spin-state x. The polarization bias is given by $\varepsilon_0 = p_\uparrow - p_\downarrow = \tanh\left(\frac{\hbar\gamma B}{2K_B T}\right)$, where B is the magnetic field, γ is the particle-dependent gyromagnetic constant,[1] K_B is Boltzmann's coefficient, and T is the thermal heat-bath temperature. Let $\varepsilon = \frac{\hbar\gamma B}{2K_B T}$ such that $\varepsilon_0 = \tanh\varepsilon$. For high temperatures or small biases, higher powers of ε can be neglected, so we approximate $\varepsilon_0 \approx \varepsilon$. Typical values of ε_0 for nuclear spins (at room temperature and a magnetic field of ~ 10 Tesla) are $10^{-5} - 10^{-6}$.

A major challenge in the application of NMR techniques is to enhance sensitivity by overcoming difficulties related to the Signal-to-Noise Ratio (SNR). Five fundamental approaches were traditionally suggested for improving the SNR of NMR. Three straightforward approaches - cooling the entire system, increasing the magnetic field, and using a larger sample - are all expensive and limited in applicability, for instance they are incompatible with live samples. Furthermore, such approaches are often impractical due to sample or hardware limitations. A fourth approach - repeated sampling - is very feasible and is often employed in NMR experiments. However, an improvement of the SNR by a factor of M requires M^2 repetitions (each followed by a significant delay to allow relaxation), making this approach time-consuming and overly costly. Furthermore, it is inadequate for samples which evolve over the averaged time-scale, for slow-relaxing spins, or for non-Gaussian noise.

1.2 Effective Cooling of Spins

The fifth fundamental approach to the SNR problem consists of cooling the spins without cooling the environment, an approach known as "effective cooling" of

[1] This constant, γ, is thus responsible for the difference in the equilibrium polarization bias of different spins [e.g., a hydrogen nucleus is about 4 times more polarized than a ^{13}C nucleus, but less polarized by three orders of magnitude than an electron spin].

the spins [6,7,8,9]. The effectively-cooled spins can be used for spectroscopy until they relax to thermal equilibrium. The following calculations are done to leading order in ε_0 and are appropriate for $\varepsilon_0 \ll 1$. A spin temperature at equilibrium is $T \propto \varepsilon_0^{-1}$. The single-spin Shannon entropy is $H = 1 - \left(\varepsilon_0^2/\ln 4\right)$. A spin temperature out of thermal equilibrium is similarly defined (see for instance [10]). Therefore, increasing the polarization bias of a spin beyond its equilibrium value is equivalent to cooling the spin (without cooling the system) and to decreasing its entropy.

Several more recent approaches are based on the creation of very high polarizations, for example dynamic nuclear polarization [11], para-hydrogen in two-spin systems [12], and hyperpolarized xenon [13]. In addition, there are other spin-cooling methods, based on general unitary transformations [7] and on (closely related) data compression methods in closed systems [8].

One method for effective cooling of spins, *reversible polarization compression (RPC)*, is based on entropy manipulation techniques. RPC can be used to cool some spins while heating others [7,8]. Contrary to conventional data compression,[2] RPC techniques focus on the low-entropy spins, namely those that get colder during the entropy manipulation process. RPC, also termed "molecular-scale heat engine", consists of reversible, in-place, lossless, adiabatic entropy manipulations in a closed system [8]. Therefore, RPC is limited by the second law of thermodynamics, which states that entropy in a closed system cannot decrease, as is also stated by Shannon's source coding theorem [4]. Consider the total entropy of n uncorrelated spins with equal biases, $H(n) \approx n(1 - \varepsilon_0^2/\ln 4)$. This entropy could be compressed into $m \geq n(1 - \varepsilon^2/\ln 4)$ high entropy spins, leaving $n - m$ extremely cold spins with entropy near zero. Due to preservation of entropy, the number of extremely cold spins, $n - m$, cannot exceed $n\varepsilon_0^2/\ln 4$. With a typical $\varepsilon_0 \sim 10^{-5}$, extremely long molecules ($\sim 10^{10}$ atoms) are required in order to cool a single spin to a temperature near zero. If we use smaller molecules, with $n \ll 10^{10}$, and compress the entropy onto $n - 1$ fully-random spins, the entropy of the remaining spin satisfies [2]

$$1 - \varepsilon_{\text{final}}^2 \geq n(1 - \varepsilon_0^2/\ln 4) - (n-1) = 1 - n\varepsilon_0^2/\ln 4. \tag{1}$$

Thus, the polarization bias of the cooled spin is bounded by

$$\varepsilon_{\text{final}} \leq \varepsilon_0\sqrt{n}\ . \tag{2}$$

When all operations are unitary, a stricter bound than imposed by entropy conservation was derived by Sørensen [7]. In practice, due to experimental limitations, such as the efficiency of the algorithm, relaxation times, and off-resonance effects, the obtained cooling is significantly below the bound given in eq 2.

Another effective cooling method is known as *polarization transfer (PT)*[6,14]. This technique may be applied if at thermal equilibrium the spins to be used for

[2] Compression of data [4] such as bits in a computer file, can be performed by condensation of entropy to a minimal number of high entropy bits, which are then used as a compressed file.

spectroscopy (the observed spins) are less polarized than nearby auxiliary spins. In this case, PT from the auxiliary spins to the observed spins is equivalent to cooling the observed spins (while heating the auxiliary spins). PT from one spin to another is limited as a cooling technique, because the polarization bias increase of the observed spin is bounded by the bias of the highly polarized spin. PT is regularly used in NMR spectroscopy, among nuclear spins on the same molecule [6]. As a simple example, consider the 3-bit molecule trichloroethylene (TCE) shown in Fig. 1. The hydrogen nucleus is about four times more polarized

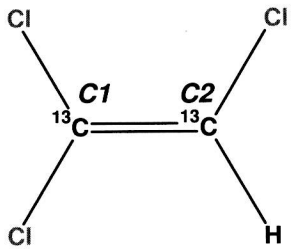

Fig. 1. *A 3-bit computer: a TCE molecule labeled with two* ^{13}C. TCE has three spin nuclei: two carbons and a hydrogen, which are named C1, C2 and H. The chlorines have a very small signal and their coupling with the carbons is averaged out. Therefore, TCE acts as a three-bit computer. The proton can be used as a reset spin because relative to the carbons, its equilibrium bias is four times greater, and its thermalization time is much shorter. Based on the theoretical ideas presented in [2], the hydrogen of TCE was used to cool both carbons, decrease the total entropy of the molecule, and bypass Shannon's bound on cooling via RPC [5].

than each of the carbon nuclei; PT from a hydrogen can be used to cool a single carbon by a factor of four. A different form of PT involves shifting entropy from nuclear spins to electron spins. This technique is still under development [9,13], but has significant potential in the future.

Unfortunately, the manipulation of many spins, say $n > 100$, is a very difficult task, and the gain of $\sqrt{n}$ in polarization is not substantial enough to justify putting this technique into practice.

In its most general form, RPC is applied to spins with different initial polarization biases, thus PT is a special case of RPC. We sometimes refer to both techniques and their combination as *reversible algorithmic cooling.*

2 Algorithmic Cooling

Boykin, Mor, Roychowdhury, Vatan, and Vrijen (hereinafter referred to as BMRVV), coined the term *Algorithmic Cooling (AC)* for their novel effective-cooling method [1]. AC expands previous effective-cooling techniques by exploiting entropy manipulations in *open systems.* It combines RPC with relaxation (namely, thermalization) of the *hotter spins*, in order to cool far beyond Shannon's entropy bound.

AC employs slow-relaxing spins (which we call *computation spins*) and rapidly relaxing spins (*reset spins*), to cool the system by pumping entropy to the environment. Scheme 1 details the three basic operations of AC. The ratio $R_{relax-times}$, between the spin-lattice relaxation times of the computation spins and the reset spins, must satisfy $R_{relax-times} \gg 1$, to permit the application of many cooling steps to the system.

In all the algorithms presented below, we assume that the relaxation time of each computation spin is sufficiently large, so that the entire algorithm is completed before the computation spins lose their polarization.

The practicable algorithmic cooling (PAC) suggested in [2] indicated a potential for near-future application to NMR spectroscopy [3]. In particular, it presented an algorithm (named PAC2) which uses any odd number of spins such that one of them is a reset spin and the other $2L$ spins are computation spins. PAC2 cools the spins such that the coldest one can (ideally) reach a bias of $(3/2)^L$. This proves an exponential advantage of AC over the best possible reversible algorithmic cooling, as reversible cooling techniques (e.g., of refs [7] and [8]) are limited to a bias improvement factor of $\sqrt{n}$. As PAC2 can be applied to small L (and small n), it is potentially suitable for near future applications.

Scheme 1: *AC is based on the combination of three distinct operations:*

1. *RPC. Reversible Polarization Compression steps redistribute the entropy in the system so that some computation spins are cooled while other computation spins become hotter than the environment.*
2. *SWAP. Controlled interactions allow the hotter computation spins to adiabatically lose their entropy to a set of reset spins, via PT from the reset spins onto these specific computation spins.*
3. *WAIT. The reset spins rapidly thermalize, conveying their entropy to the environment, while the computation spins remain colder, so that the entire system is cooled.*

2.1 Block-Wise Algorithmic Cooling

The original Algorithmic Cooling (BMRVV AC) [1] was designed to address the scaling problem of NMR quantum computing. Thus, a significant number of spins are cooled to a desired level and arranged in a consecutive block, such that the entire block may be viewed as a register of cooled spins. The calculation of the cooling degree attained by the algorithm was based on the law of large numbers, yielding an exponential reduction in spin temperature. Relatively long molecules were required due to this statistical nature, in order to ensure the cooling of 20, 50, or more spins (the algorithm was not analyzed for a small number of spins). All computation spins were assumed to be arranged in a linear chain where each computation spin (e.g., ^{13}C) is attached to a reset spin (e.g., ^{1}H). Reset and computation spins are assumed to have the same bias ε_0. BMRVV AC consists of applying a recursive algorithm repeating (as many times as necessary) the sequence of RPC, SWAP (with reset spins), and WAIT, as detailed in Scheme 1. The relation between gates and NMR pulse sequences is discussed in ref [15].