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FINITE-TIME THERMODYNAMICS AND SIMULATED ANNEALING

BJARNE ANDRESEN

*Ørsted Laboratory, University of Copenhagen
Universitetsparken 5, DK-2100 Copenhagen Ø
Denmark*

Abstract.

Finite-time thermodynamics is the extension of traditional reversible thermodynamics to include the extra requirement that the process in question goes to completion in a specified finite length of time. As such it is by definition a branch of irreversible thermodynamics, but unlike most other versions of irreversible thermodynamics, finite-time thermodynamics does not require or assume any knowledge about the microscopics of the processes, since the irreversibilities are described by macroscopic constants such as friction coefficients, heat conductances, reaction rates and the like. Some concepts of reversible thermodynamics, such as potentials and availability, generalize nicely to finite time, others are completely new, e.g. endoreversibility and thermodynamic length. The basic ideas of finite-time thermodynamics are reviewed and several of its procedures presented, emphasizing the importance of power.

The global optimization algorithm simulated annealing was designed for extremely large and complicated systems and therefore inspired by analogy to statistical mechanics. Its basic version is outlined, and several notions from finite-time thermodynamics are introduced to improve its performance. Among these are an optimal temperature path, the use of ensembles, and an analytic two-state model with Arrhenius kinetics.

1. INTRODUCTION

1.1 Motivation

From its infancy over 150 years ago thermodynamics has provided limits on work or heat exchanged during real processes. The first problem treated in a systematic way was how much work a steam engine can produce from the burning of one ton of coal. With true scientific generalization Sadi Carnot concluded that any engine taking in heat from a hot reservoir at temperature T_H

has to deposit some of that heat in a cold reservoir (e.g. the surroundings), whose temperature we call T_L . The largest fraction of the heat which can be converted into work is

$$\eta_C = 1 - \frac{T_L}{T_H}, \quad (1.1)$$

traditionally known as the Carnot efficiency. This expression contains the two basic ingredients of a thermodynamic limit: (i) it applies to *any* process converting heat into work; and (ii) it is an *absolute* limit, i.e. no process, however ingenious, can do better.

As thermodynamic theory developed, emphasis changed from process variables like work and heat exchanged to state variables like entropy and chemical potential. A bridge between the two are the thermodynamic work potentials, such as Helmholtz free energy F for isothermal, isochoric processes or the Gibbs free energy G for isothermal, isobaric processes. They are defined such that, under the given conditions, their changes provide upper bounds on the work a process can supply or lower bounds on the work required to drive a process. Gibbs introduced the concept of ‘available work’ as the maximum work that can be extracted from a system allowed to go from a constrained, internally equilibrated state to a state in equilibrium with its surroundings. This quantity is used more and more frequently in engineering contexts [1, 2] under the names ‘availability’ in the U.S. and ‘exergy’ in Europe. For a system relaxing to an ambient temperature T_0 , pressure P_0 , and chemical potentials μ_{0i} it is given by

$$A = U + P_0V - T_0S - \sum_i \mu_{0i}N_i \quad (1.2)$$

and is thus not a state function in the usual sense of depending only on variables of the system; the availability depends on the intensive variables of the environment as well.

Such criteria of merit have long been common currency for thermodynamic studies in physics, chemistry, and engineering. They all share one characteristic: The ideal to which any real process is compared is a *reversible process*. Stated in a different way, *traditional thermodynamics is a theory about equilibrium states and about limits on process variables for transformations from one equilibrium state to another*. Nowhere does time enter the formulation, so these limits must be the lossless, reversible processes which proceed infinitely slowly and thus take infinite length of time to complete. However, referring back to the original question addressed by Carnot, who is interested in an engine which operates in-

finitely slowly (and thus produces zero power) — or any other process with zero rate of operation, for that matter?

In order to obtain more realistic limits to the performance of real processes *finite-time thermodynamics is designed as the extension of traditional thermodynamics to deal with processes which have explicit time or rate dependencies.* These constraints, of course, imply a certain amount of loss, or entropy production, which is at the heart of the question posed above.

1.2 Early developments

In the course of developing finite-time thermodynamics we discovered that a few isolated papers already had considered different aspects of processes operating at nonzero rates. The first of these was the important work of Tolman and Fine [3] who put the Second Law of thermodynamics into equality form,

$$W = \Delta A - T_0 \int_{t_i}^{t_f} \dot{S}_{\text{tot}} dt \quad (1.3)$$

by subtracting the work equivalent of the entropy produced during the process from the reversible work, i.e. the decrease of system availability, as defined in eq. (1.2). The superscript dot indicates rate, and the integral limits are the initial and final times of the process. This is a quantification of the ‘price of haste’.

Another model has evolved into almost a classic paradigm of systems operating in finite time. This is the model of Curzon and Ahlborn [4], a Carnot engine with the simple constraint that it be linked to its surroundings through *finite* heat conductances. Figure 1 illustrates the slightly more general endoreversible system with the triangle signifying any reversible engine. (The term endoreversible means ‘internally reversible’, i.e. all irreversibilities reside in the coupling of flows to the surroundings. In this case the irreversibilities are the resistance to heat transfer and possibly friction.) It turns out that the results derived by Curzon and Ahlborn explicitly for an interior Carnot engine are equally valid for a general endoreversible system. The maximum efficiency of their engine is of course $\eta_C = 1 - T_L/T_H$, obtained at zero rate so that losses across the resistors vanish, but these authors showed that, when the system operates to produce *maximum power*, the efficiency of the engine is only

$$\eta_w = 1 - \sqrt{\frac{T_L}{T_H}} . \quad (1.4)$$

Besides the simplicity of the expression it is remarkable that it does not contain the value of the heat conductances.

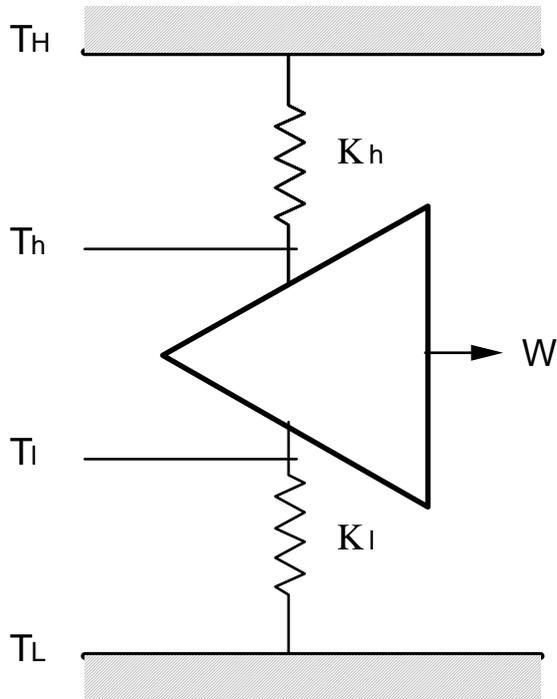


Figure 1. An endoreversible engine has all its losses associated with its coupling to the environment, there are no internal irreversibilities. This is illustrated here as resistances in the flows of heat to and from the working device indicated by a triangle. These unavoidable resistances cause the engine proper to work across a smaller temperature interval, $[T_h; T_l]$ than that between the reservoirs, $[T_H; T_L]$, one which depends on the rate of operation.

2. PERFORMANCE BOUND WITHOUT PATH

The smallest amount of information one can ask for concerning the performance of a system is a single number, e.g. the work or heat exchanged during the process, its efficiency, or any other figure of merit. In most cases this can be calculated without knowledge of the detailed path followed and is then computationally much simpler to obtain.

2.1 Generalized potentials

In traditional thermodynamics potentials are used to describe the ability of a system to perform some kind of work under given constraints. These constraints are usually the constancy of some state variables like pressure, volume, temperature, entropy, chemical potential, particle number, etc. Under such conditions the decrease in thermodynamic potential P from state i to state f is equal to the amount of work that is produced when a reversible process carries out the transition, and hence is the upper bound to the amount of work produced by any other process,

$$W \leq W_{\text{rev}} = P_i - P_f. \quad (2.1)$$

In this section we will show that the constraints need not simply be the constancy of some state variable, and that the potentials may be generalized to contain constraints involving time [5]. The procedure will be a straight forward extension of the Legendre transformations [6] used in traditional thermodynamics [7, 8], and we will start with such an example.

In a reversible process heat and work can be expressed as inexact differentials,

$$dQ = TdS, \quad dW = PdV, \quad (2.2)$$

i.e. they cannot by themselves be integrated, further constraints defining the integration path are required. Such a constraint could be that the process is isobaric, $dP = 0$. One can then add a suitable integrating zero-term, $x dP$ to make dW an exact differential. The obvious choice is $x = V$,

$$dW = PdV = PdV + VdP = d(PV), \quad (2.3)$$

such that the isobaric work potential becomes $P = PV$. Similarly the isobaric heat potential $U + PV$ is obtained from

$$dQ = TdS = dU + PdV = dU + PdV + VdP = d(U + PV), \quad (2.4)$$

where the combined First and Second Laws of thermodynamics

$$dU = TdS - PdV \quad (2.5)$$

have been used.

Now, the constraints need not be the constancy of one of the state variables. Consider a balloon with constant surface tension α . In equilibrium with an external pressure P_{ex} such a sphere of radius r has an internal pressure

$$P = P_{\text{ex}} + \frac{2\alpha}{r}, \quad (2.6)$$

which can be rearranged into

$$(P - P_{\text{ex}})V^{1/3} = 2\alpha \left(\frac{4\pi}{3} \right)^{1/3}. \quad (2.7)$$

Since the right hand side of this equation is a constant, this means that $(P - P_{\text{ex}})V^{1/3}$ is an integral of motion for the fluid inside the balloon. We can then add a suitable amount of $d[(P - P_{\text{ex}})V^{1/3}] (=0)$ to dW to make it exact [see eq. (2.11) below for how to do it],

$$\begin{aligned} dW &= PdV = PdV + \frac{3}{2} V^{2/3} d[(P - P_{\text{ex}})V^{1/3}] \\ &= d\left[\frac{1}{2} V(3V - P_{\text{ex}})\right]. \end{aligned} \quad (2.8)$$

Thus the work done by the coupled system, surface + fluid, is given by the decrease in the potential $P = \frac{1}{2} V(3V - P_{\text{ex}})$, regardless of path followed.

In its most general form the Legendre transformation can be used to calculate a potential P for the arbitrary process variable B , expressible as a path integral in terms of generalized forces f_i and displacements x_i ,

$$B = \sum_i \int f_i dx_i = \int \mathbf{f} \cdot d\mathbf{x}; \quad (2.9)$$

B will usually be work, and vector notation is used for compactness. To find P , one adds to $\mathbf{f} \cdot d\mathbf{x}$ an integrating term $\mathbf{g} \cdot d\mathbf{y}$, where $d\mathbf{y}$ is necessarily zero as a result of the constraints defining the process. Note that $d\mathbf{y} = \mathbf{0}$ may involve time and could come from a condition in the form of a differential equation as well as from the more familiar thermodynamic condition of a constant variable, as used in the example above. Hence the differential form $d\mathbf{y} = \mathbf{0}$ is used rather than the integrated form $\mathbf{y} = \text{constant}$, since \mathbf{y} itself may not exist. The mathematical problem of finding P has two steps, finding a function \mathbf{g} which makes $d\omega = \mathbf{f} \cdot d\mathbf{x} + \mathbf{g} \cdot d\mathbf{y}$ an exact differential dP , and then integrating to get P itself. The first step involves the Cauchy-Riemann condition that $d\omega$ has equal cross derivatives with respect to the free state variables, e.g. a and b :

$$\frac{\partial}{\partial b} \left[\mathbf{f} \cdot \left(\frac{\partial \mathbf{x}}{\partial a} \right)_b + \mathbf{g} \cdot \left(\frac{\partial \mathbf{y}}{\partial a} \right)_b \right] = \frac{\partial}{\partial a} \left[\mathbf{f} \cdot \left(\frac{\partial \mathbf{x}}{\partial b} \right)_a + \mathbf{g} \cdot \left(\frac{\partial \mathbf{y}}{\partial b} \right)_a \right] \quad (2.10)$$

or

$$\left(\frac{\partial \mathbf{g}}{\partial a} \right)_b \cdot \left(\frac{\partial \mathbf{y}}{\partial b} \right)_a - \left(\frac{\partial \mathbf{g}}{\partial b} \right)_a \cdot \left(\frac{\partial \mathbf{y}}{\partial a} \right)_b = \left(\frac{\partial \mathbf{f}}{\partial b} \right)_a \cdot \left(\frac{\partial \mathbf{x}}{\partial a} \right)_b - \left(\frac{\partial \mathbf{f}}{\partial a} \right)_b \cdot \left(\frac{\partial \mathbf{x}}{\partial b} \right)_a. \quad (2.11)$$

With \mathbf{f} , $d\mathbf{x}$, and $d\mathbf{y}$ known, this is the equation from which \mathbf{g} may be obtained. In the usual case of $\mathbf{f} = P$, $d\mathbf{x} = dV$, $a = V$, and $b = P$, the right hand side of eq. (2.11)

simplifies to 1. The second step in finding P , the integration of dP , is, of course, only unique within a constant of the motion; i.e. two methods of integration may yield two different potentials P and P' , but their variations will always be the same, $\Delta P = \Delta P'$.

2.2 Thermodynamic length

In an effort to develop a more direct and transparent way of calculating all the usual partial derivatives in traditional thermodynamics Weinhold [9–13] proposed using scalar products between vectors in the abstract space of equilibrium states of a system, represented by all its extensive variables X_i . The products were defined relative to

$$\mathbf{M}_U = \left\{ \frac{\partial^2 U}{\partial X_i \partial X_j} \right\} \quad (2.12)$$

as the metric, where U is the internal energy. However, second derivatives are usually identified as curvatures and, as such, should be interpreted as availabilities in Gibbs space (U as a function of all the other extensive variables). This lead us to seek another interpretation of pathlengths calculated with Weinhold's metric, now called thermodynamic lengths, and we [14] found that they are always changes in some molecular velocities, depending, of course, on the constraints of the process (isobaric, isochoric, etc.).

Subsequently Salamon and Berry [15] found a connection between the thermodynamic length along a process path and the (reversible) availability lost in the process. Specifically, if the system moves via states of local thermodynamic equilibrium from an initial equilibrium state i to a final equilibrium state f in time τ , then the dissipated availability $-\Delta A$ is bounded from below by the square of the distance (i.e. length of the shortest path) from i to f times ε/τ , where ε is a mean relaxation time of the system. If the process is endoreversible, the bound can be strengthened to

$$-\Delta A \geq \frac{L^2 \varepsilon}{\tau}, \quad (2.13)$$

where L is the length of the *traversed* path from i to f . Equality is achieved at constant thermodynamic speed $v = dL/dt$ corresponding to a temperature evolution given by [16, 17]

$$\frac{dT}{dt} = -\frac{vT}{\varepsilon\sqrt{C}}, \quad (2.14)$$

where C is the heat capacity of the system. For comparison, the bound from traditional thermodynamics is only

$$-\Delta A \geq 0. \quad (2.15)$$

An analogous expression exists for the total entropy production during the process:

$$\Delta S^u \geq \frac{L^2 \varepsilon}{\tau}. \quad (2.16)$$

The length L is then calculated relative to the entropy metric

$$\mathbf{M}_S = - \left\{ \frac{\partial^2 S}{\partial X_i \partial X_j} \right\} \quad (2.17)$$

which (when expressed in identical coordinates!) is related to \mathbf{M}_U by [18]

$$\mathbf{M}_U = -T_0 \mathbf{M}_S, \quad (2.18)$$

where T_0 as usual is the environment temperature. In statistical mechanics, where entropy takes the form

$$S(\{p_i\}) = - \sum_i p_i \ln p_i, \quad (2.19)$$

the metric \mathbf{M}_S is particularly simple, being the diagonal matrix [19]

$$\mathbf{M}_S = - \left\{ \frac{1}{p_i} \right\}. \quad (2.20)$$

The same procedure of calculating metric bounds for dynamic systems has been applied to coding of messages [20] and to economics [21].

More recently [22] we have relaxed a number of the assumptions in the original work, primarily those restricting the system to be close to equilibrium at all times and the average form of the relaxation time ε . The more general bound replacing eq. (2.16) then becomes

$$\Delta S^u \geq \frac{1}{\Xi} \left(\int_{\xi_i}^{\xi_f} \frac{1}{T\sqrt{C}} \left| \frac{dU}{d\xi} \right| \sqrt{1 + \frac{\theta}{CT} \frac{dU}{d\xi} + \dots} d\xi \right)^2 \quad (2.21)$$

with $\Xi = \xi_f - \xi_i$ being the total duration of the process in natural dimensionless time units,

$$d\xi = dt/\varepsilon(T), \quad (2.22)$$

and where we have defined

$$\theta(T) = 1 + \frac{T}{2C} \frac{\partial C}{\partial T}. \quad (2.23)$$

The equality (lower bound) in eq. (2.21) is achieved when the integrand is a constant, i.e. when

$$\frac{dS^u}{d\xi} = \text{constant}. \quad (2.24)$$

Consequently, constant rate of entropy production, when expressed in terms of natural time, is the path or operating strategy which produces the least overall entropy.

One can express the optimal path, eq. (2.24), in a form similar to eq. (2.14):

$$\frac{dT}{dt} \sqrt{1 + \frac{\theta(T) \varepsilon (dT/dt)}{T}} + \dots = \text{constant} \times \frac{T}{\varepsilon\sqrt{C}}. \quad (2.25)$$

The constant thermodynamic speed algorithm, eq. (2.14), is thus the leading term of the general solution in an expansion about equilibrium behavior.

3. OPTIMAL PATH

3.1 Optimal path calculations

A knowledge of the maximum work that can be extracted during a given process, e.g. calculated by one of the procedures described in the previous section, may not by itself be sufficient. One may also want to know *how* this maximum

work can be achieved, i.e. the time path of the thermodynamic variables of the system. The primary tool for obtaining this path is optimal control theory.

This is not the place to repeat the mechanics of optimal control calculations (see e.g. [23–25]). Let it suffice to point out that in order to set up the optimal control problem one must specify

- the controls, i.e. the variables that can be manipulated by the operator (they may be a volume, rate, voltage, heat conductance, etc.);
- limits on the controls and on the state variables, if any (in order to avoid unphysical situations such as negative temperatures and infinite speeds);
- the equations that govern the time evolution of the system (they will usually be differential equations describing heat transfer rates, chemical reaction rates, friction, and other loss mechanisms);
- the constraints that are imposed on the system (e.g. conserved quantities, the quantities held constant, or any requirements on reversibility. The constraints may either be differential, instantaneous i.e. algebraic, or integral i.e. not obeyed at each point but over the entire interval);
- the desired quantity to be maximized, called the objective function (usually expressed as an integral); and finally
- whether the duration of the process is fixed or part of the optimization.

Typical manipulation usually leads to a set of coupled, non-linear differential equations for which a qualitative analysis and a numerical solution are the only hope. Thus answering the more demanding question about the optimal time path rather than the standard question about maximum performance requires a considerably larger computational effort. On the other hand, once the time path is calculated, all other thermodynamic quantities may be calculated from it, much like the wave function is the basis of all information in quantum mechanics.

3.2 Criteria of performance

Efficiency, the earliest criterion of performance for engines, measured how much water could be pumped out of a mine by burning a ton of coal. Other familiar criteria include effectiveness (efficiency relative to the Carnot efficiency), change of thermodynamic potential, and loss of availability, all of which are measures of work. Potentials for heat can also be defined (see Sect. 2.1) but are less common, and we have used the minimization of entropy production in a separate study [26].

The Curzon-Ahlborn analysis and most of our own analyses use a quite different criterion, that of *power*. This quantity is of course zero for any revers-

ible system, and maximizing power forces us to deal with systems operating at finite rates. Other criteria of performance are the rate of entropy production and the rate of loss of availability. Entropy production was a function introduced in the earliest thinking about irreversible thermodynamics [27–30], but more from the differential, local, instantaneous viewpoint than from the global, integral view of entire optimized processes. Under some circumstances, optimizing one of these quantities is equivalent to optimizing another. For example, minimizing the entropy production is equivalent to minimizing the loss of availability, at least in those cases in which the irreversibilities can be represented as spontaneous heat flows [26].

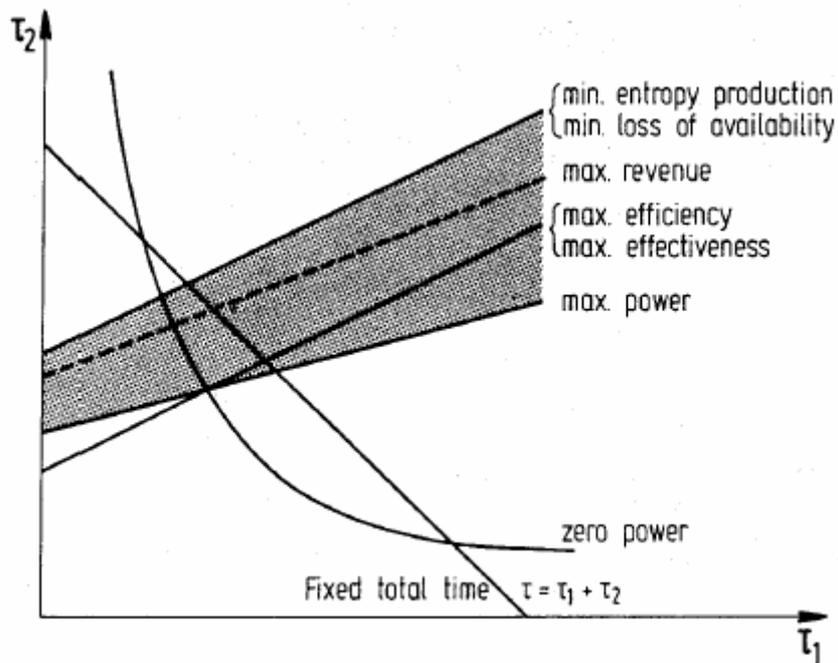


Figure 2. If an endoreversible engine (Fig. 1) spends time τ_1 in contact with the hot reservoir and τ_2 in contact with the cold reservoir, the optimal proportioning between τ_1 and τ_2 depends on what one chooses to optimize, as indicated. The locus of maximum revenue for a power producing system falls in the shaded area for any choice of prices, as described in the text. Only contact times above the hyperbola marked 'zero power' actually correspond to positive power production.

Salamon and Nitzan [31] have optimized the Curzon-Ahlborn engine for a number of these objective functions. Assuming the working fluid to be in contact with the hot reservoir for the period τ_1 and the cold reservoir for the period τ_2 , the optimal time distributions are shown in Fig. 2. The diagonal $\tau = \tau_1 + \tau_2$ indicates fixed total cycle time, and only processes above the curve labeled 'zero

power' produce positive power. It is quite obvious that different criteria of merit dictate different operating conditions for the process. Even when not knowing the precise objective function but only that it belongs to a specified class, one can sometimes say a good deal about the possible optimal behavior of the system. If one considers the Curzon-Ahlnorn engine to be a model of a power plant which buys heat q (coal) at the unit price α and sells work w (electricity) at the unit price β , its net revenue is $\Pi = \beta w - \alpha q$. All solutions to the problem of maximizing this revenue are bounded on one side by the solutions to the maximum power problem (when α is significant compared to β) and on the other side by the solutions corresponding to minimum loss of availability (when coal and electricity are priced according to their availability contents). While this is a very simple example, this approach has far reaching possibilities for describing biological, ecological, and economic systems.

4. SIMULATED ANNEALING

Simulated annealing is a global optimization procedure [32] which exploits an analogy between combinatorial optimization problems and the statistical mechanics of physical systems. The analogy gives rise to an algorithm for finding near-optimal solutions to the given problem by simulating the cooling of the corresponding physical system. Just as nature, under most conditions, manages to cool a macroscopic system into or very close to its ground state in a short period of time even though its number of degrees of freedom is of the order of Avogadro's number, so does simulated annealing rapidly find a good guess of the solution of the posed problem.

Even though the original class of problems under consideration [32] was combinatorial optimization, excellent results have been obtained with seismic inversion [33], pattern recognition [34], and neural networks [35] as well, just to name a few. Since layout and scheduling problems in computer and telecommunications systems frequently contain elements of combinatorial optimization, and their complexity often rivals and even surpasses that of a mole of chemical substance, simulated annealing is excellently suited to attack those problems. The virtue of simulated annealing is its efficiency as a general-purpose method for handling extremely complicated problems for which no direct solution method is known without the need for developing an ad hoc algorithm.

4.1 The algorithm

The simulated annealing algorithm is based on the Monte Carlo simulation of physical systems. It requires the definition of a state space $\Omega = \{\omega\}$ with an

associated cost function (physical analog: energy) $E: \Omega \rightarrow \mathbb{R}$ which is to be minimized in the optimization. At each point of the Monte Carlo random walk in the state space the system may make a jump to a neighboring state; this set of neighbors, known as the move class $N(\omega)$, must of course also be specified. Alternatively one may specify the complete transition probability matrix \mathbf{P} between all states of the system. The only control parameter of the algorithm is the temperature T of the heat bath in which the corresponding physical system is immersed, measured in energy units, i.e. we take Boltzmann's constant $k = 1$.

The random walk inherent in the Monte Carlo simulation is accomplished by the Metropolis algorithm [36] which states that:

- (i) At each step t of the algorithm a neighbor ω' of the current state ω_t is selected at random from the move class $N(\omega_t)$ to become the candidate for the next state.
- (ii) It actually becomes the next state only with probability

$$P_{\text{accept}} = \begin{cases} 1 & \text{if } \Delta E \leq 0 \\ e^{-\Delta E/T_t} & \text{if } \Delta E > 0 \end{cases}, \quad (4.1)$$

where $\Delta E = E(\omega') - E(\omega_t)$ is the increase in cost for the move. If this candidate is accepted, then $\omega_{t+1} = \omega'$.

The only thing left to specify is the sequence of temperatures T_t appearing in the Boltzmann factor in P_{accept} , the so-called annealing schedule. Like in metallurgy, this cooling rate has a major influence on the final result. A quench is quick and dirty, often leaving the system stranded in metastable states high above the ground state/optimal solution. Slow annealing produces the best result but is computationally expensive.

This completes the formal definition of the simulated annealing algorithm, which in principle simply is repeated numerous times until a satisfactory result is obtained.

4.2 The optimal annealing schedule

So far all suggested simulated annealing temperature paths (annealing schedules) have been of the a priori type and thus have not adjusted to the actual behavior of the system as the annealing progresses. Examples of such schedules are

$$T(t) = a e^{-t/b} \quad (4.2)$$

$$T(t) = \frac{a}{b+t} \tag{4.3}$$

$$T(t) = \frac{a}{\ln(b+t)} \cdot \tag{4.4}$$

The real annealing of physical systems often has rough parts where the surrounding temperature must be decreased slowly due to phase transitions or regions of large heat capacity or slow internal relaxation. The same behavior is seen in the abstract systems, so annealing schedules which take such variations into account are preferable in order to keep computation time at a minimum for a given accuracy of the final result [37].

At this point I would like to make the analogy between the abstract simulated annealing process and a real thermodynamic process even stronger. Specifically, if the correspondence with statistical mechanics implied in the simulated annealing procedure involving phase space and state energies is valid, then further results from thermodynamics will probably also carry over to simulated annealing.

Since asking a question (= one evaluation of the energy function) in information theoretic terms is equivalent to producing one bit of entropy, the computationally most efficient procedure will be the temperature schedule $T(t)$ which overall produces minimum entropy. Above we have derived various bounds and optimal paths for real thermodynamic systems using finite-time thermodynamics [15, 19, 26, 38]. The minimum-entropy production path which most readily generalizes to become the optimal simulated annealing schedule, is the one calculated with thermodynamic length [cf. eq. (6.4) below]:

$$\frac{dT}{dt} = - \frac{vT}{\epsilon\sqrt{C}} \tag{2.14}$$

or equivalently

$$\frac{\langle E \rangle - E_{\text{eq}}(T)}{\sigma} = v. \tag{4.5}$$

As long as the system in question is accurately described by statistical mechanics, these bounds and the paths that achieve them will provide the most efficient solution within the allotted time. Since the layout of major networks and the allocation of access to common scarce resources are closely related to graph partitioning, simulated annealing with a constant thermodynamic speed schedule should yield good results. In these expressions v is the (constant) thermodynamic speed, C and ϵ are the heat capacity and internal relaxation time

of the system, respectively, $\langle E \rangle$ and σ the corresponding mean energy and standard deviation of its natural fluctuations, and finally $E_{\text{eq}}(T)$ is the internal energy the system would have if it were in equilibrium with its surroundings at temperature T . The physical interpretation of eq. (4.5) is that the environment should at all times be kept v standard deviations ahead of the system. Similarly eq. (2.14) indicates that the annealing should slow down where internal relaxation is slow and where large amounts of ‘heat’ has to be transferred out of the system [17]. In case C and ε do not vary with temperature, eq. (2.14) integrates to the standard schedule eq. (4.2). The more realistic assumption of an Arrhenius-type relaxation time, $\varepsilon \sim \exp(a/T)$, and a heat capacity $C \sim T^{-2}$ implies the vastly slower schedule eq. (4.4). Reality is usually in between these extremes. Figure 3 shows the successive decrease in energy for annealings on a graph partitioning problem following different annealing schedules.

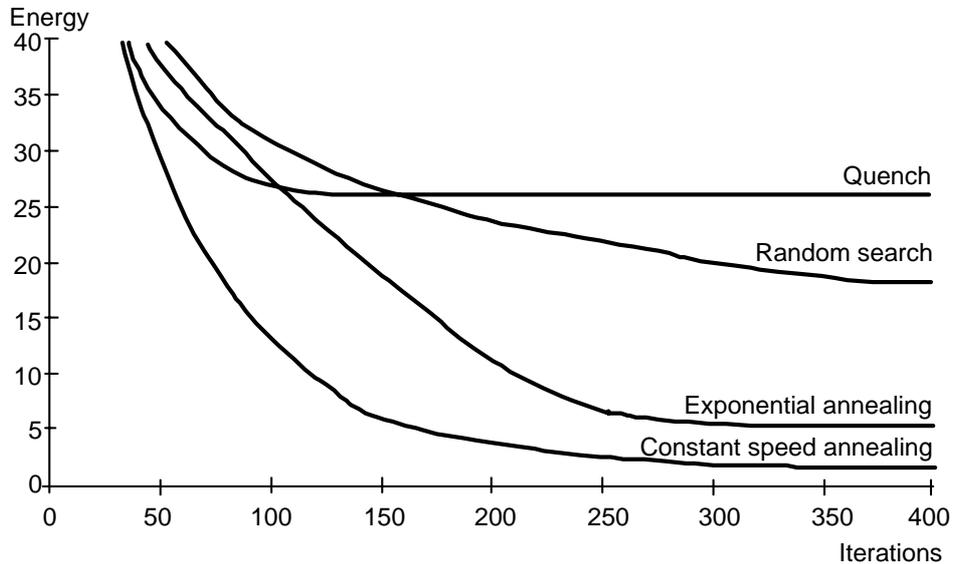


Figure 3. Energy for a graph partitioning problem as the annealing progresses, using different annealing schedules: quench ($T=0$), random search ($T=\infty$), exponential (eq. (4.2)), constant speed (eq. (2.14) or (4.5)).

4.3 Parallel implementation

The extra temperature dependent variables of the constant thermodynamic speed schedule of course require additional computational effort. Since systems often change considerably in a few steps, ergodicity is not fulfilled, so the use of time averages to obtain $\langle E \rangle$, σ , C , and ε is usually not satisfactory. Instead we suggest [39] running an ensemble of systems in parallel, i.e. with the same annealing schedule, in the true spirit of the analogy to statistical mechanics.

Then these variables can be obtained anytime as ensemble averages based on the system degeneracies $p_i = p(E_i)$:

$$Z(T) = \sum_i p_i \exp(-E_i/T) \quad (4.6)$$

$$E(T) = T^2 \frac{d \ln Z}{dt} \quad (4.7)$$

$$C(T) = \frac{dE}{dT} = \frac{\langle (\Delta E)^2 \rangle}{T^2} \quad (4.8)$$

$$\varepsilon(T) = \frac{-1}{\ln \lambda_2} \approx \frac{T^2 C(T)}{\sum_i p_i \sum_{j>i} (E_j - E_i)^2 P_{ji} \exp(-E_i/T)}, \quad (4.9)$$

where λ_2 is the second largest eigenvalue of the thermalized version of the transition probability matrix \mathbf{P} among all the energy levels ($\lambda_1 = 1$ corresponds to equilibrium).

But from where does one get the degeneracies p_i ? Actually [39], information to calculate the temperature-independent (or infinite-temperature, if you prefer) transition probability matrix \mathbf{P} can be accumulated during the annealing run by simply adding up in a matrix \mathbf{Q} the number of attempted moves (not just the accepted ones) from level i to j as the calculation progresses. Normalization of \mathbf{Q} yields a good estimate of \mathbf{P} ,

$$P_{ji} = Q_{ji} / \sum_k Q_{ki}. \quad (4.10)$$

The degeneracies \mathbf{p} are then the eigenvector of \mathbf{P} corresponding to the eigenvalue 1.

This use of ensemble annealing is particularly well suited for implementation on present day parallel computers. A further analysis of its performance has been carried out by Ruppeiner, Pedersen, and Salamon [40], and the trade-off between ensemble size and duration of annealing for fixed total computation cost has been addressed by Pedersen et al. [41].

4.4 An analytic model

The procedure outlined above with a continuous compilation of statistical data about the system under investigation can be quite computation intensive.

To alleviate that we have found [42] that the assumption of a simple two-state model, equivalent to the one-dimensional Ising model [43], is a good approximation to the microscopic picture of a number of complex optimization problems. (This approximation is used only for determining the optimal temperature schedule $T(t)$; the annealing itself is carried out with the full energy function.) The combinatorial necklace or integrated circuit problem [17, 39, 40], partitioning of random graphs [44], and certain spin glass systems [45] are obvious candidates for the model, since they involve individual vertices which can be placed in either of two sets. In general the two-state model should be useful for any system consisting of a set of weakly interacting two-level systems.

The model states that each particle can be in one of two states only: a lower state of energy $-J$ and a higher state of energy $+J$. For ease of notation we define the dimensionless temperature variable

$$x = \frac{T}{2J} . \quad (4.11)$$

From the partition function for a macroscopic system comprised of N such particles ($N \gg 1$) at temperature x the system energy and heat capacity follow directly:

$$E(x) = -NJ \tanh \frac{1}{2x} \quad (4.12)$$

$$C(x) = \frac{N \left(\frac{1}{2x}\right)^2}{\cosh^2 \frac{1}{2x}} . \quad (4.13)$$

In addition we assume that the system relaxation time is well represented by the classical Arrhenius expression

$$\epsilon(x) = A \exp(B/x), \quad (4.14)$$

where A is a (constant) collision frequency, and B is the apparent barrier height of the transition state. Even though the energy landscape of the system will generally contain several different barriers, only the highest will be effective in the long-time limit when all the faster relaxations have died out, i.e. close to equilibrium. This assumption is consistent with the derivation of eq. (2.14).

Introducing these assumptions into the optimal rate annealing schedule eq. (2.14) yields

$$\frac{dx}{dt} = -v' x^2 \left(\exp\left(\frac{1}{x}\right) + 1 \right) \exp\left(-\frac{B+1/2}{x}\right), \quad (4.15)$$

where v' is a constant. This is the differential equation defining the optimal temperature path $x(t)$ for a two-state model with an Arrhenius-type relaxation. It can, at least in principle, be solved analytically before any annealing begins and thus replaces the much more time consuming procedure of collecting statistical information along the way presented in the previous section [39]. The 'price' for this faster procedure clearly is less generality and required knowledge about the system in advance.

5. SUMMARY

Finite-time thermodynamics was 'invented' in 1975 by R. S. Berry, P. Salamon, and myself as a consequence of the first world oil crisis. It simply dawned on us that all the existing criteria of merit were based on reversible processes and therefore were totally unrealistic for most real processes. That made an evaluation of the potential for improvement of a given process quite difficult.

Finite-time thermodynamics is developed from a macroscopic point of view with heat conductances, friction coefficients, overall reaction rates, etc. rather than based on a microscopic knowledge of the processes involved. Consequently most of the ideas of traditional thermodynamics have been assimilated, e.g. the notions of thermodynamic potential (Sect. 2.1) and availability. At the same time we have seen new concepts emerge, e.g. the non-equivalence of well-honored criteria of merit (Sect. 3.2), the importance of power as the objective (Sect. 1.2 and 3.2), the generality of the endoreversible engine, and in particular thermodynamic length (Sect. 2.2). Several of these abstract concepts have been successfully applied to practical optimizations [46–52].

Lately the notions and results of finite-time thermodynamics, at times in connection with statistical mechanics and information theory, have been used to perfect the global optimization method simulated annealing (Sect. 4). However, the surface has only been scratched, there is still plenty of room for inspiration from such well-known concepts as state entropy, free energy, and transition state theory. Simulated annealing has proven to be a very useful general purpose optimization algorithm for extremely complicated problems, even with fixed temperature schedules, eqs. (4.2) – (4.4). Elaborating the analogy to physical statistical mechanical systems with the introduction of optimality results from finite-time thermodynamics has improved the efficiency of the algorithm noticeably, and the use of ensembles of random walkers has made it self-adapt-

ing. Finally, a simple analytical model based on the one-dimensional Ising model may reduce the computational time considerably.

The method as described above mimics nature as it equilibrates systems on an atomic or molecular scale (e.g. chemical reactions or crystal structures). Inspiration can also be lifted from nature's way of developing the most favorable systems on the macroscopic biological scale: evolution. Several annealing procedures based on evolution with its cloning of successful species and dying out of unsuccessful ones have been developed as replacements for the Metropolis algorithm of Sect. 4.1, notably by Ebeling and coworkers [53–55] and by Schuster [56]. In my opinion the two lines of thought are complementary in the sense that they are advantageous for many trials and for a more limited set of tests, respectively.

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