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Computing via material topology optimisation

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ABSTRACT

We construct logical gates via topology optimisation (aimed to solve a station problem of heat conduction) of a conductive material layout. Values of logical variables are represented by high and low values of a temperature at given sites. Logical functions are implemented via the formation of an optimum layout of conductive material between the sites with loading conditions. We implement AND and XOR gates and a one-bit binary half-adder.

1. Introduction

Any programmable response of a material to external stimulation can be interpreted as computation. To implement a logical function in a material one must map space–time dynamics of an internal structure of a material onto a space of logical values. This is how experimental laboratory prototypes of unconventional computing devices are made: logical gates, circuits and binary adders employing interaction of wave-fragments in light-sensitive Belousov–Zhabotinsky media [1], swarms of soldier crabs [2], growing lamellipodia of slime mould *Physarum polycephalum* [3], crystallisation patterns in "hot ice" [4], peristaltic waves in protoplasmic tubes [5]. In many cases logical circuits are 'built' or evolved from a previously disordered material [6], e.g. networks of slime mould *Physarum polycephalum* [7], bulks of nanotubes [8], nano particle ensembles [9,10]. In these works the computing structures could be seen as growing on demand, and logical gates develop in a continuum where an optimal distribution of material minimised internal energy. A continuum exhibiting such properties can be coined as a "self-optimising continuum". Slime mould of *Physarum polycephalum* well exemplifies such a continuum: the slime mould is capable of solving many computational problems, including mazes and adaptive networks [11]. Other examples of the material behaviour include bone remodelling [12], roots elongation [13], sandstone erosion [14], crack and lightning propagation [15], growth of neurons and blood vessels, etc. Some other physical systems suitable for computations were also proposed in [6,16–18]. In all these cases, a phenomenon of the formation of an optimum layout of material is related to non-linear laws of material behaviour, resulting in the evolution of material structure governed by algorithms similar to those used in a topology optimisation of structures [19]. We develop the ideas of material optimisation further and show, in numerical models, how logical circuits can be build in a conductive material self-optimise its structure governed by configuration of inputs and outputs.

The paper is structured as follows. In Section 2 we introduce topology optimisation aimed to solve a problem of a stationary heat conduction. In Section 3 we describe the algorithm parameters for the considered cases. Gates AND and XOR are designed and simulated in Sections 4 and 5. We design one-bit half-adder in Section 6. Directions of further research are outlined in Section 7.

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2. Topology optimisation

A topology optimisation in continuum mechanics aims to find a layout of a material within a given design space that meets specific optimum performance targets [20–22]. The topology optimisation is applied to solve a wide range of problems [23], e.g. maximisation of heat removal for a given amount of heat conducting material [24], maximisation of fluid flow within channels [25], maximisation of structure stiffness and strength [23], development of meta-materials satisfying specified mechanical and thermal physical properties [23], optimum layout of plies in composite laminates [26], the design of an inverse acoustic horn [23], modelling of amoeboid organism growing towards food sources [27], optimisation of photonics-crystal band-gap structures [28].

A standard method of the topology optimisation employs a modelling material layout that uses a density of material, ρ, varying from 0 (absence of a material) to 1 (presence of a material), where a dependence of structural properties on the density of material is described by a power law. This method is known as Solid Isotropic Material with Penalisation (SIMP) [29]. An optimisation of the objective function consists in finding an optimum distribution of ρ: $\min_{\rho} f(\rho)$.

The problem can be solved in various numerical schemes, including the sequential quadratic programming (SQP) [30], the method of moving asymptotes (MMA) [31], and the optimality criterion (OC) method [23]. The topology optimisation problem can be replaced with a problem of finding a stationary point of an ordinary differential equation (ODE) [19]. Considering density constraints on ρ, the right term of ODE is equal to a projection of the negative gradient of the objective function. Such optimisation approach is widely used in the theory of projected dynamical systems [32]. Numerical schemes of topology optimisation solution can be found using simple explicit Euler algorithm. As shown in [33] iterative schemes match the algorithms used in bone remodelling literature [34].

In this work the topology optimisation problem is applied to heat conduction problems [35]. Consider a region in the space Ω with a boundary $\Gamma = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$, separated for setting the Dirichlet (D) and the Neumann (N) boundary conditions. For the region Ω we consider the steady-state heat equation given in:

$$\nabla \cdot k\nabla T + f = 0 \text{ in } \Omega \tag{1}$$

$$T = T_0 \text{ on } \Gamma_D \tag{2}$$

$$(k\nabla T) \cdot n = Q_0 \text{ on } \Gamma_N \tag{3}$$

where T is a temperature, k is a heat conduction coefficient, f is a volumetric heat source, and n is an outward unit normal vector. At the boundary Γ_D a temperature $T = T_0$ is specified in the form of Dirichlet boundary conditions, and at the boundary Γ_N of the heat flux $(k\nabla T) \cdot n$ is specified using Neumann boundary conditions. The condition $(k\nabla T) \cdot n = 0$ specified at the part of Γ_N means a thermal insulation (adiabatic conditions).

When stating topology optimisation problem for a solution of the heat conduction problems it is necessary to find an optimal distribution for a limited mass of conductive material M in order to minimise heat release, which corresponds to designing a thermal conductive device. It is necessary to find an optimum distribution of material density ρ within a given area Ω in order to minimise the cost function:

$$\text{Minimise } C(\rho) = \int_{\Omega} \nabla T \cdot (k(\rho)\nabla T) \tag{4}$$

$$\text{Subject to } \int_{\Omega} \rho \le M \tag{5}$$

In accordance with the SIMP method the region being studied can be divided into finite elements with varying material density ρ_i assigned to each finite element i. A relationship between the heat conduction coefficient and the density of material is described by a power law as follows:

$$k_i = k_{\min} + (k_{\max} - k_{\min})\rho_i^p, \qquad \rho_i \in \lfloor 0, 1 \rfloor \tag{6}$$

where k_i is a value of heat conduction coefficient at the ith finite element, ρ_i is a density value at the ith element, $k_{\max}$ is a heat conduction coefficient at $\rho_i = 1$, $k_{\min}$ is a heat conduction coefficient at $\rho_i = 0$, p is a penalisation power ($p > 1$).

In order to solve the problems (1)–(6) we apply the following techniques used in the dynamic systems modelling. Assume that ρ depends on a time-like variable t. Let us consider the following differential equation to determine density in ith finite element, ρ_i, when solving the problem stated in (1)–(6) [19]:

$$\dot{\rho_i} = \lambda\left(\frac{pC_i(\rho_i)}{\rho_i} - \mu V_i\right), \qquad C_i(\rho_i) = \int_{\Omega_i} \nabla T \cdot (k_i(\rho)\nabla T)d\Omega \tag{7}$$

where dot above denotes the derivative with respect to t, Ω_i is a domain of ith finite element, V_i is a volume of ith element, λ is a physical dimensional positive constant, μ is a positive parameter that regulates the relative importance of the cost function (4) and mass constraint (5). This equation can be obtained by applying methods of the projected dynamical systems [19,33] or bone remodelling methods [34,36]. It should be noted that term $\frac{pC_i(\rho_i)}{\rho_i}$ is the derivative of the compliance with

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