

## DETERMINATION OF FREE ENERGIES ON A SIMULATION MODEL

Josip Kasač\*

Department of Robotics and Automation of Manufacturing Systems,  
Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb,  
Zagreb, Croatia

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### SUMMARY

Social free energy was recently introduced as a measure of social action obtainable from a given social system, without changes in its structure. In this article its relation with physical free energy for a toy-model of interacting agents is analysed. Values of the social and physical free energies are equivalent for the case of quasi-stationary state of toy-model of interacting agents.

### KEY WORDS

social free energy, social entropy, social systems, agent, modelling

### CLASSIFICATION

ACM Categories and subject descriptors: J.4 [Computer Applications]; Social and behavioral sciences - Sociology

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\* $\eta$ : [josip.kasac@fsb.hr](mailto:josip.kasac@fsb.hr); +385 1 6168 375; Department of Robotics and Automation of Manufacturing Systems, Faculty of Mechanical Engineering and Naval Architecture, I. Lučića 1, HR-10000 Zagreb, Croatia

## 1. INTRODUCTION

Modelling of social systems based on notions developed in theoretical physics develops rapidly. Within that approach, the social meaning of free energy has been addressed [1-4] along with related thermodynamic potentials [5]. Social free energy was introduced in a general way as a measure of system resources which are unused in regular, predicted functioning, but which are involved during suppression of environmentally induced system dynamics changes [3]. Depending on the context, it was recognized as a profit [1], a common benefit [2], or availability [4]. The free energy in the references listed was introduced with a usual physical formula, and was given a sociological interpretation. In that way the multiplicity of notions point on the one hand toward solid motivation for introduction of free energy into social context, and on the other hand that unified approach into social interpretation of physical free energy is missing.

In order to contribute to consideration of free energy as a quantity with intrinsic social meaning, it is opportune to demonstrate for a particular system the equality of independently introduced physical free energy and social free energy. That equality is demonstrated in this article in case of quasi-stationary states of an interacting agent toy-model. Agent based model is exploited in order to gain insight into the formation of macroscopic patterns through perpetual realizations of microscopic rules of interactions [6], i.e., agent-agent and agent-environment interactions.

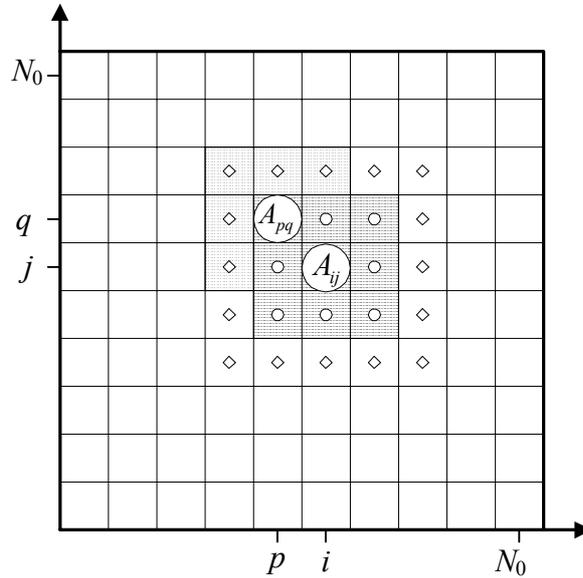
Model exploited has twofold purpose. On the one hand, it contributes to the understanding of the evolution of a system characterized by a combination of microscopic and macroscopic rules. On the other hand, characterization of its evolution in terms of physical and social free energy is emphasized. Contributions to social free energy are existing resources of a system that are not required for predicted, regular actions. In the toy model of this article that is reduced to a surplus of resources. The physical free energy is calculated using the standard, equilibrium physics expression.

The article is organized as follows. The model structure and dynamics are introduced in the second section, and model indicators in the third section. Results of model simulation are given in the fourth section, corresponding discussion in the fifth section, and summary of main results in the sixth section.

## 2. MODEL FORMULATION

The model includes mutually interacting agents, their configuration and environmental influence. Agents are located at fixed positions forming a two-dimensional net of dimensions  $N_0 \times N_0$ , Fig. 1. The agent coordinates are expressed as  $(i, j)$  and represents the  $i$ -th knot in one direction and the  $j$ -th knot in the other direction of the net. For simplicity, the agents are denoted as  $A_{ij}$ . Agent  $A_{ij}$  collects the scalar quantity  $u_{ij}(k)$ , called a resource in  $k$ -th time interval, and tries to maximize it without limits. The amount of resources owned is a positive number or zero. An agent  $A_{ij}$  with resources  $u_{ij}(k)$  is considered rich if  $u_{ij}(k) \geq u_0$  is valid, poor if  $u_0 > u_{ij}(k) > 0$  is valid, and dead if  $u_{ij}(k) = 0$ . If resources of a particular agent become negative in some time step, they are set to zero and the agent is considered dead. For a rich agent  $A_{ij}$  with resources  $u_{ij}(k)$  the difference  $u_{ij}(k) - u_0$  is called

surplus of resources. Similarly, for a poor agent with resources  $u_{ij}(k)$ , the difference  $u_0 - u_{ij}(k)$  is called lack of resources. The scalar character of resources is admissible if there exist an exchange ratio connecting all resource types. Each agent is capable of collecting unlimited amount of resources through the interaction with the environment.



**Figure 1.** Two-dimensional net with agents. Two of the agents,  $A_{ij}$  and  $A_{pq}$ , are emphasized in order to explain the principle of the agent-agent interaction. To determine the total amount of resources that the rich agent will give to the poor one, the total resources of their nearest neighbourhoods are considered. Circles denote the nearest neighbours of agent  $A_{ij}$ .

As a consequence of internal, otherwise unspecified dynamics, agents regularly consume a finite value of resources  $c$ . This value is equal for all agents.

Because of the environmental influence, agents' resources are changed for a random amount  $w_{ij}(k)$ , and in this model synchronously. The distribution of changes  $w_{ij}(k)$  is the Gaussian distribution with a mean value  $a$  and a variance  $\mu$ . The mean value  $a$  represents the average resource change, and for a system we take  $a > 0$ . In each time interval there are some resources obtained from the environment, and some resources destroyed because of the influences from the environment. If resources are smaller after the interaction with the environment this means that destructive influences, e.g., fire or flood, were stronger than the effects of making the resources larger. It has been shown that the functional representation of the resources distribution usually has a skew shape [7]. Seemingly we take here a symmetric function as a resource change distribution. However, since the positive (negative) part of the Gaussian distribution represents making the resources larger (smaller), we see that this distribution qualitatively collects the total interaction of the agents with the environment. A consequence of the Gaussian distribution considered is that the environment production is infinite.

Such a setup of the model includes the relevant agent characteristics, in accordance with the definitions of the agent [6, 8], and the social agent [9]. Each agent act on himself or herself, which is taken into account with the parameter  $c$ , and interacts with

environment, which is included through  $a$  and  $\mu$ . The agents respond to the instantaneous environment state optimally what, nevertheless, does not assure them a sufficient amount of resources. The constancy of the parameters in space means that the system latency and integrity are strong [10]. Model parameters partially cover the adaptation. It improves for higher values of  $a$ . For example, if the agents resemble units in agricultural societies, a better adaptation means a better understanding of regularities in plant growth, or animal behaviour, clear signs of understanding of a part of environment complexity [11]. If the agents are firms in a particular economy segment, then a better adaptation means more intensive paying of attention to customer needs, and resource provider potentials. In addition, a better adaptation means that rapid changes are less possible.

There is a significant overlap between the model quantities and the quantities in related theories. It is not possible to link them directly because of their presumably verbal nature. In the sociological approach compacted in the PILOTS model [7], a social system state is characterized by the meta-variable population (P), and the variables information (I), space (S), technology (T), organization (O), and level of living (L). Larger freely disseminated information content, higher technology level, better organization, and partially better level of living make parameter  $a$  larger.

The resource dynamic can be represented by

$$u_{ij}(k+1) = u_{ij}(k) + \Delta t (\text{Inflow}(i, j; k) - \text{Outflow}(i, j; k)), \quad (1)$$

where  $\text{Inflow}(i, j; k)$  is flow of resources from environment to agent,  $\text{Outflow}(i, j; k)$  is flow of resources from agent to environment, and  $\Delta t$  is time interval. Inflow and outflow can be decomposed in following way

$$\text{Inflow}(i, j; k) = w_{ij}(k) + I_{ij}(k), \quad (2)$$

$$\text{Outflow}(i, j; k) = c + O_{ij}(k), \quad (3)$$

where  $I_{ij}(k)$  is the flow of resources from neighbouring agents to the agent  $A_{ij}$  (if agent  $A_{ij}$  is poor) and  $O_{ij}(k)$  is the flow of resources from the agent  $A_{ij}$  to neighbouring agents (if agent  $A_{ij}$  is rich). More precisely, above flows can be expressed as

$$I_{ij}(k) = H(u_{ij}(k) - u_0) \sum_{p=i-1}^{i+1} \sum_{q=j-1}^{j+1} H(u_0 - u_{pq}(k)) I_{ij}^{pq}(k), \quad (4)$$

$$O_{ij}(k) = H(u_0 - u_{ij}(k)) \sum_{p=i-1}^{i+1} \sum_{q=j-1}^{j+1} H(u_{pq}(k) - u_0) O_{ij}^{pq}(k), \quad (5)$$

where

$$H(x) = \begin{cases} 0; & x \geq 0 \\ 1; & x < 0 \end{cases}, \quad (6)$$

is Heaviside step function,  $I_{ij}^{pq}(k)$  is resources flow from agent  $A_{pq}$  to agent  $A_{ij}$  (if agent  $A_{pq}$  is rich), and  $O_{ij}^{pq}(k)$  is resources flow from agent  $A_{ij}$  to agent  $A_{pq}$  (if agent  $A_{pq}$  is poor).

The amount of resources which agent  $A_{pq}$  will give to agent  $A_{ij}$  depend on following factors:

a) surplus of resources in neighbourhood of agent  $A_{ij}$ ,

$$R_{ij}(k) = \sum_{p=i-1}^{i+1} \sum_{q=j-1}^{j+1} (u_{pq}(k) - u_0) H(u_0 - u_{pq}(k)), \quad (7)$$

b) lack of resources in neighbourhood of agent  $A_{pq}$ ,

$$P_{pq}(k) = \sum_{n=p-1}^{p+1} \sum_{m=q-1}^{q+1} (u_0 - u_{nm}(k)) H(u_{nm}(k) - u_0), \quad (8)$$

c) surplus of resources of agent  $A_{pq}$ ,

$$\tilde{u}_{pq}(k) = u_{pq}(k) - u_0, \quad (9)$$

d) lack of resources of agent  $A_{ij}$ ,

$$\hat{u}_{ij}(k) = u_0 - u_{ij}(k). \quad (10)$$

So, flow  $I_{ij}^{pq}(k)$  depends on above mentioned factors

$$I_{ij}^{pq}(k) = f(R_{ij}(k), P_{pq}(k), \tilde{u}_{pq}(k), \hat{u}_{ij}(k)). \quad (11)$$

A possible choice of this function is based on following reasoning. If agent  $A_{pq}$  is only rich agent in neighbourhood of agent  $A_{ij}$ , then he or she assigns own surplus of resources to agent  $A_{ij}$  proportionally to rate between lack of resources of agent  $A_{ij}$  and lack of resources in neighbourhood of agent  $A_{pq}$ ,

$$\bar{I}_{ij}^{pq}(k) = \frac{\hat{u}_{ij}(k) \tilde{u}_{pq}(k)}{P_{pq}(k) \cdot 2}, \quad (12)$$

(factor  $1/2$  ensure that agent  $A_{ij}$  couldn't has more resources then agent  $A_{pq}$  in next time interval). If agent  $A_{pq}$  is not only rich agent in neighbourhood of agent  $A_{ij}$ , then previous amount of resources will be multiplied by rate between surplus of resources of agent  $A_{pq}$  and surplus of resources in neighbourhood of agent  $A_{ij}$ ,

$$I_{ij}^{pq}(k) = \frac{\tilde{u}_{pq}(k)}{R_{ij}(k)} \bar{I}_{ij}^{pq}(k), \quad (13)$$

or, finally

$$I_{ij}^{pq}(k) = \frac{\hat{u}_{ij}(k) \tilde{u}_{pq}(k) \tilde{u}_{pq}(k)}{P_{pq}(k) R_{ij}(k) \cdot 2}. \quad (14)$$

Similarly, the amount of resources which agent  $A_{ij}$  will give to agent  $A_{pq}$  depend on following factors:

a) surplus of resources in neighbourhood of agent  $A_{pq}$ ,

$$R_{pq}(k) = \sum_{n=p-1}^{p+1} \sum_{m=q-1}^{q+1} (u_{nm}(k) - u_0) H(u_0 - u_{nm}(k)), \quad (15)$$

b) lack of resources in neighbourhood of agent  $A_{ij}$ ,

$$P_{ij}(k) = \sum_{p=i-1}^{i+1} \sum_{m=j-1}^{j+1} (u_0 - u_{pq}(k)) H(u_{pq}(k) - u_0), \quad (16)$$

c) surplus of resources of agent  $A_{ij}$ ,

$$\tilde{u}_{ij}(k) = u_{ij}(k) - u_0, \quad (17)$$

d) lack of resources of agent  $A_{pq}$ ,

$$\hat{u}_{pq}(k) = u_0 - u_{pq}(k). \quad (18)$$

Outflow  $O_{ij}^{pq}(k)$  depends on above mentioned factors on similar way as for inflow  $I_{ij}^{pq}(k)$ ,

$$O_{ij}^{pq}(k) = \frac{\hat{u}_{pq}(k)}{P_{ij}(k)} \frac{\tilde{u}_{ij}(k)}{R_{pq}(k)} \frac{\tilde{u}_{ij}(k)}{2}. \quad (19)$$

### 3. INDICATORS

States of the model are generally, physically non-stationary states. However, in a special case of  $a = c$ , the resources average net transfer is zero, hence there is a stationary resource flow of intensity equal  $a$ . Non-stationarity is then a consequence of a variable number of agents. When, furthermore, such a change is relatively small, an almost stationary situation occurs.

Indicators attributed to a system state are heterogeneous. One set of them originates in physics: entropy  $S$ , temperature denoted here as  $T$ , and physical free energy  $F$ . Other indicators are more similar to social indicators: number of agents  $N$ , and surplus of resources. The formulas for indicator determination are written having in mind restrictions of their validity induced by non-stationarity.

Entropy is calculated using

$$S = -N \int_0^{\infty} p(u) \ln p(u) du, \quad (20)$$

where  $p(u)$  is numerically determined distribution of agent resources. It is taken that (20) gives the values of both physical and social entropy. That is not always valid [7]. Here it is a consequence of only one type of resources and the measure associated with it. In more complex models, several types of resources are explicitly treated, hence there is need to differentiate e.g., material and information flows [7].

Temperature is introduced through the relation

$$T = \left( \frac{\partial U}{\partial S} \right)_{V, N, q}, \quad (21)$$

in which  $V, N, q$  are constant space, number of agents and flow from environment to a system. Here, temperature is calculated during system evolution as

$$T = \left( \frac{\partial U}{\partial S} \right)_V. \quad (22)$$

The internal energy is the sum of individual agent resources

$$U = \sum_{i=1}^{N_0} \sum_{j=1}^{N_0} u_{ij}(k), \quad (23)$$

so that the physical free energy of a system, given by

$$F = U - TS, \quad (24)$$

may be determined using (20), (22) and (23). Additionally, we consider the surplus

$$F_s = \sum_{i=1}^{N_0} \sum_{j=1}^{N_0} H(u_0 - u_{ij}(k))(u_{ij}(k) - u_0), \quad (25)$$

which we call social free energy, and compare it with (24). The social free energy (25) is amount of resources that the agents could disseminate in accordance with (4) and (5).

## 4. RESULTS AND DISCUSSION

We concentrate on the case  $a \approx c$  because of two reasons. The formal reason is that both for  $a$  much larger or much smaller than  $c$  the dynamics is trivial, realized either as total flourishing or total collapse of a system, respectively. The conceptual reason is that when  $a \approx c$ , one expects that the latency of a model will be large enough, so that the parameters used in the model could be considered constant. Then the states significantly resemble stationary states, and the equations (20-23) are highly appropriate. In case  $a = c$  system adaptation is maximal, because there are no unused environment resources like for  $a < c$ , while the efficiency of use of obtained resources is not maximal in the case  $a > c$ . Additionally, in this article the level of consumption  $c$  is considered equal to the reference level  $u_0$ .

The model dynamics is simulated during 100 time units from the initial moment what satisfies the assumed constancy of model parameters.

In Fig. 2 the time dependence of number of rich, poor, and dead agents is given for  $a/c$  equal to 0.8, 0.9, and 0.99. It is seen that the changes in number of alive agents become negligible after several time units. Then the system is equilibrated in the sense that the influence of the initial state ceased, and the gradual collapse of the system is not clearly seen.

The distribution of resources among agents is shown in Fig. 3. All graphs shown contain one maximum and a localized tail on the side of high resources.

The time dependence of total resources is shown in Fig. 4, while the time dependence of physical and social free energies are shown in Fig. 5.

One can express the difference between the fitting functions for physical and social free energies by integrating the squared relative difference of these two functions in the time interval in which the form (22) is applicable. Since there is no preferred

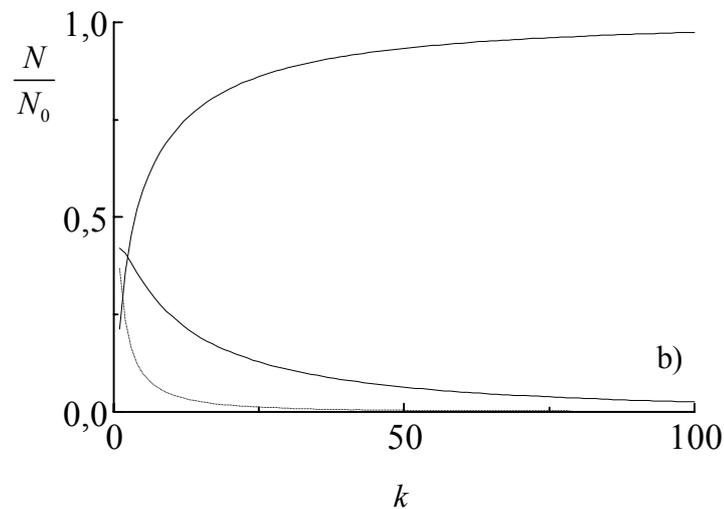
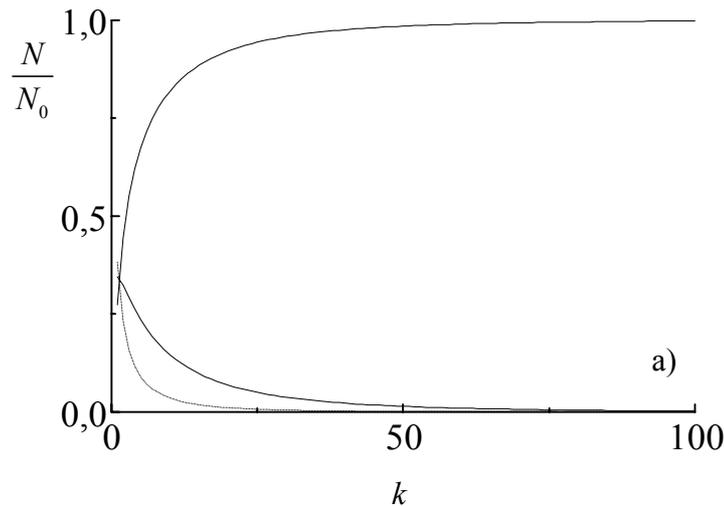
function between two of these, their difference is compared with their arithmetic mean in obtaining the relative value. The difference function is taken to be

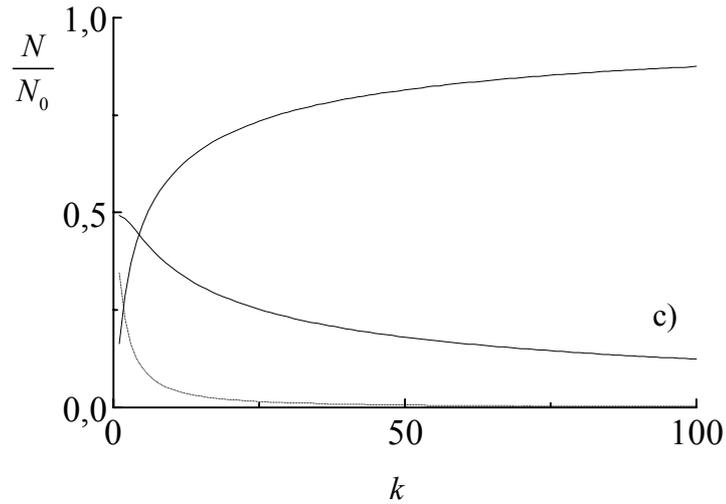
$$D(a/c) \equiv \int_{30}^{80} \left| \frac{F_s(t) - F(t)}{[F_s(t) + F(t)]/2} \right|^2 dt. \quad (26)$$

Its dependence on  $a/c$  is shown in Figure 6. The conditions in (26) are that relaxation of initial state, and long-time dynamics are excluded from integration range, which is why it is restricted from  $t = 30$  to  $t = 80$ . Relatively small changes of  $D$ , caused by small changes of integration limits, are therefore admissible.

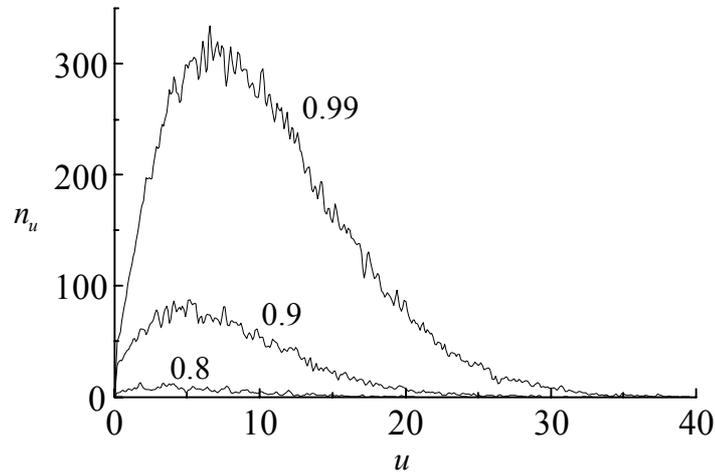
The minimum of the relative difference between the free energies  $D$ , attained for  $a = c$  contributes to the statement that  $F$  and  $F_s$  have equal values. In case  $a = c$  the system behaviour is expected to be the closest to the equilibrium one. Fig. 6 shows that the alignment between the  $F$  and  $F_s$  is the largest in the case in which the equilibrium physics approach has the largest applicability.

In a more developed model, in which there are explicit mechanisms for changes the values of the defined parameters, the purposefulness of a system development could be introduced. Then the transfer of additional resources related to other purposes could be defined. Such transfers could contribute to internal system development, relatively independently of the environment.

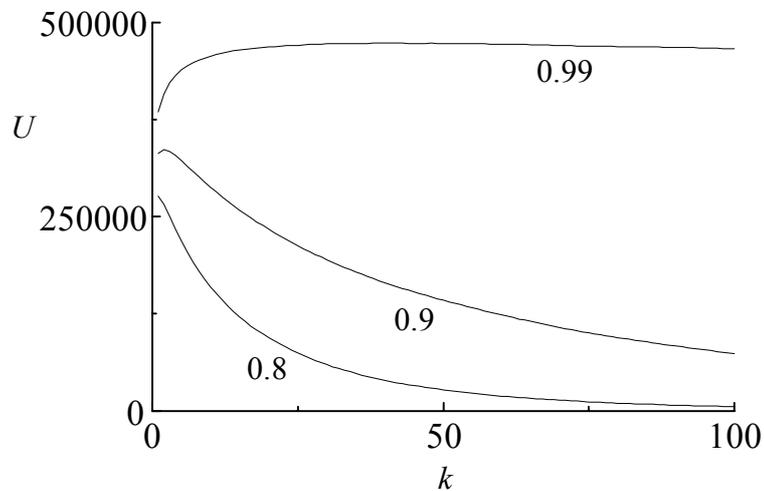




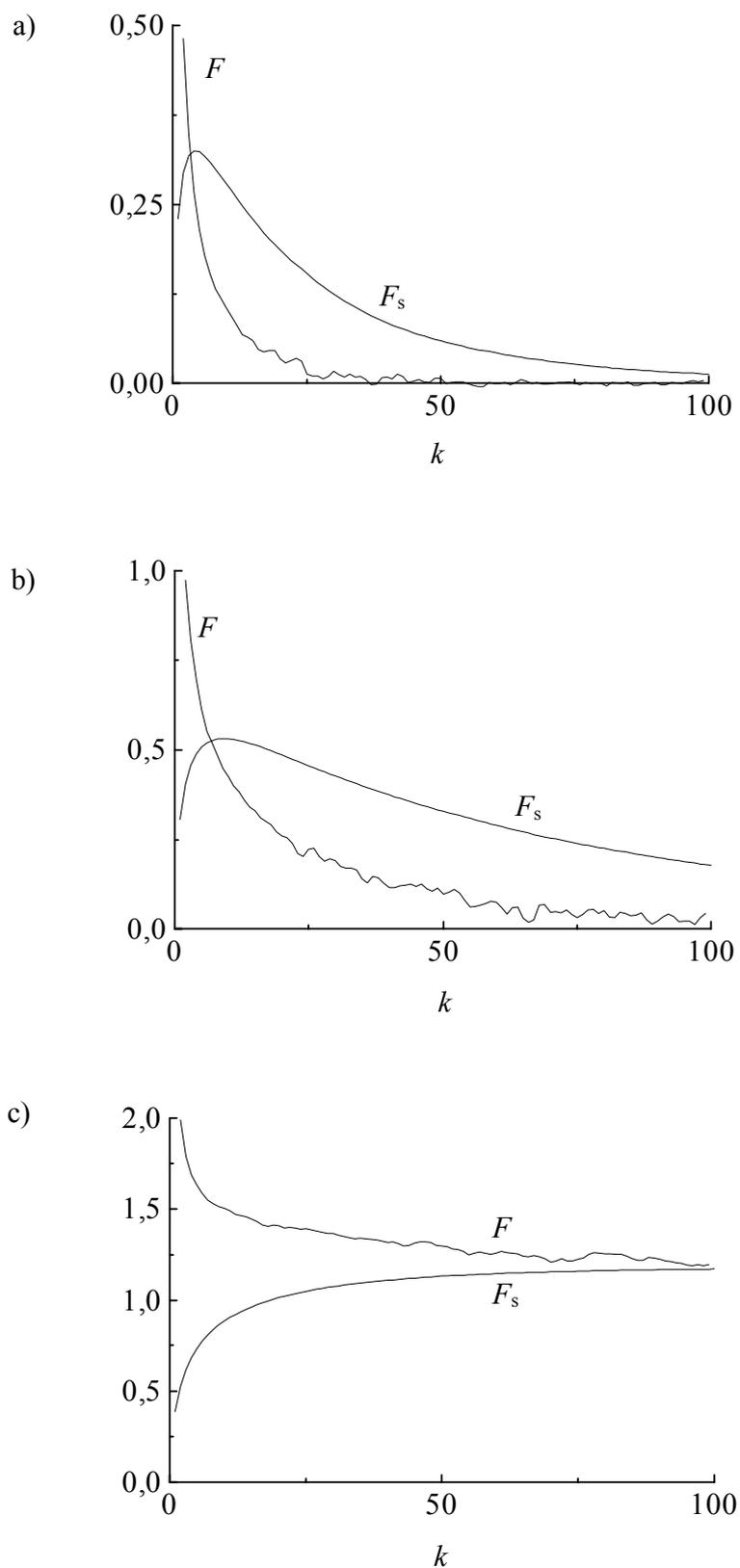
**Figure 2.** Time dependence of a number of agents in the system, for  $a/c$  equal to a) 0.8, b) 0.9, and c) 0.99. Dashed line – number of poor agents. Full lines denote the number of dead (rise in time) and alive (fall in time) agents. The initial number of agents is  $N_0 = 40000$ .



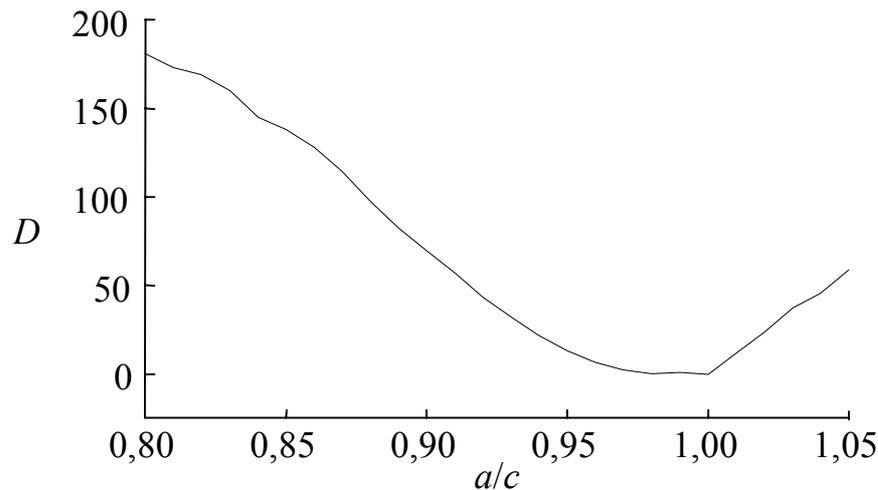
**Figure 3.** Distribution of resources among agents in time unit  $k = 100$ . Numbers in the graph are values of  $a/c$ .



**Figure 4.** Time dependence of total resources  $U$ . Numbers in the graph are values of  $a/c$ .



**Figure 5.** Time dependence of thermodynamic free energy  $F$  and social free energy  $F_s$  for  $a/c$  equal to a) 0.8, b) 0.9, and c) 0.99.



**Figure 6.** Dependence of the difference (26) between thermodynamic and social free energy on  $a/c$ . This graph shows that the best numerical consistency of thermodynamic and social free energy is for the stationary thermodynamic state, where our approach is supposed to work best.

## 5. SUMMARY AND CONCLUSIONS

In this article the relation between the social and physical free energies is analyzed numerically, using toy model simulation. In the model, the interacting agents in a stochastic environment are interpreted from the physical and sociological point of views.

The physical free energy is shown to be equal to the social free energy in case of quasi-stationary states. Furthermore, free energy in this model has a clear meaning of surplus of resources. Despite the relatively restricted class of states for which the equality of the two free energies is shown, because of the different time dependence of their fitting functions, it is conjectured that physical and social free energy are different representations of the same function.

In further work on this model more profiled forms of thermodynamic functions, e.g., Gibbs energy, are to be used in order to incorporate a variable number of agents. In addition, the intrasystem generation of new agents is to be included. In this case, the truly stationary states are possible bringing about the possibility of testing the equality of free energies in a broader class of states.

## 6. ACKNOWLEDGMENTS

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## Određivanje slobodnih energija na simulacijskom modelu

Josip Kasač

Zavod za robotiku i automatizaciju proizvodnih sustava,  
Fakultet strojarstva i brodogradnje, Sveučilište u Zagrebu,  
Zagreb, Hrvatska

### SAŽETAK

Socijalna slobodna energija uvedena je kao mjera socijalne akcije dobivene u danom socijalnom sustavu, bez promjene njegove strukture. U ovom radu analizira se njena veza sa fizikalnom slobodnom energijom na primjeru jednostavnog modela interagirajućih agenata. Vrijednosti socijalne i fizikalne slobodne energije su ekvivalentne u slučaju kvazistacionarnog stanja modela interagirajućih agenata.

### KLJUČNE RIJEČI

socijalna slobodna energija, socijalna entropija, socijalni sustavi, agenti, modeliranje