Speed-gradient principle for description of transient dynamics in systems obeying maximum entropy principle

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Abstract. The speed-gradient variational principle (SG-principle) for nonstationary nonequilibrium systems is formulated and illustrated by an example. It is proposed to use the SG-principle to model transient (relaxation) dynamics for systems satisfying maximum entropy principle. Nonstationary processes generated with the method of dynamics of particles are studied. A comparison of theoretic prediction and simulation results confirming reasonable prediction precision is presented.

Keywords: Variational principles, Maximum Entropy Principle, method of particles
PACS: 02.70.Ns;89.70.Cf

INTRODUCTION

The equations of motion for physical systems are often derived from variational principles: principle of least action, maximum entropy principle, etc. [1, 2]. Variational principles are based on specification of a functional (usually, integral functional) and determination of real motions as points in an appropriate functional space providing extrema of the specified functional. The principle is called integral if the functional to be extremized has an integral form.

In addition to integral principles, differential (local) ones were proposed: Gauss principle of least constraint, principle of minimum energy dissipation and others. It has been pointed out by M. Planck [3] that the local principles have some preference with respect to integral ones because they do not fix dependence of the current states and motions of the system on its later states and motions. In 1957 E.T. Jaynes formulated the Maximum Entropy Principle (MEP): the entropy of any physical system tends to increase until it achieves its maximum value under constraints imposed by other physical laws [4]. Such a prediction in implicit form can be found in the works of W. Gibbs.

In [5, 6] a new local evolution principle, so called **speed-gradient (SG) principle** originated from the SG-design method of nonlinear control theory [7, 8] was proposed and illustrated by a number of examples from mechanics. In [10] SG-principle was extended to the case of systems with constraints.

This paper is aimed at application of the SG-principle to entropy-driven systems. First, the formulation of the SG-principle is recalled. Then the SG-principle is applied to derivation of transient dynamics for a system driven by maximum entropy principle and its simulation results are compared with those for molecular dynamics method.

SPEED-GRADIENT VARIATIONAL PRINCIPLE

Consider a class of physical systems described by systems of differential equations

$$\dot{x} = f(x,u,t), \tag{1}$$

where $x = (x_1,\ldots,x_n)^T$ is n-dimensional column vector of the system state (^{T} is the transposition sign), $u = (u_1,\ldots,u_m)^T$ is m-dimensional column vector of free (input) variables, $\dot{x} = dx/dt$, $t \geq 0$. The problem of modelling system dynamics can be posed as the search of a law of change of $u(t)$ meeting some criterion of "natural", or "reasonable" behavior of the system. Let such a behavior be specified as a tendency to achieve a goal, specified as decreasing the value of the *goal functional* $Q(x)$, where $Q(x)$ is given *a priori*. The choice of $Q(x)$ should reflect physical essence of the problem and it is critical for the result. An ultimate goal may be also introduced as achievement of the minimum value of Q(x):

$$Q(x(t)) \to 0 \ \text{ as } \ t \to \infty, \tag{2}$$

if a nonnegative $Q(x)$ is chosen: $Q(x) \geq 0$.

The first step of the speed-gradient procedure is to calculate the speed $\dot{Q} = \frac{dQ}{dt} = \omega(x,u,t)$, where $\omega(x,u,t) = \frac{\partial Q(x)}{\partial x} f(x,u,t)$. The second step is to evaluate the gradient of the speed $\nabla_u \dot{Q}$ with respect to input vector u (speed-gradient vector). Finally the law of dynamics is formed as the feedback law in the *finite form*

$$u = -\gamma \nabla_u \dot{Q}(x,u,t). \tag{3}$$

or in the *differential form*

$$\frac{du}{dt} = -\gamma \nabla_u \dot{Q}(x,u,t), \tag{4}$$

where $\gamma > 0$ is a positive scalar or a positive definite symmetric matrix *gain* (positivity of a matrix is understood as positive definiteness of associated quadratic form). The underlying idea of the choices (3) or (4) is that the motion along the antigradient of the speed $\dot{Q}$ provides decrease of $\dot{Q}$. It may eventually lead to negativity of $\dot{Q}$ which, in turn, yields decrease of Q. Under some natural assumptions achievement of the ultimate goal (2) can be derived as a mathematical statement [5, 8] which is, however, beyond the theme of this paper. The speed-gradient principle is formulated as follows.

Speed-gradient principle: *Among all possible motions of the system only those are realized for which the input variables change proportionally to the speed gradient $\nabla_u \dot{Q}(x,u)$ of an appropriate goal functional $Q(x)$. If there are constraints imposed on the system motion, then the speed-gradient vector should be projected onto the set of admissible (compatible with constraints) directions.*

According to the SG-principle, to describe a system dynamics one needs to introduce the goal function $Q(x)$. The choice of $Q(x)$ should reflect the tendency of natural behavior to decrease the current value $Q(x(t))$. Systems obeying the SG-principle will be called *SG-systems*. In this paper only the models (1) in a special form are considered:

$$\dot{x} = u, \tag{5}$$

i.e. a law of change of the state velocities is sought.

Since gradient of a function is the direction of it maximum growth, the SG-direction is the direction of maximum growth for $\dot{Q}(x,u,t)$, i.e. direction of maximum production rate for Q. Respectively, the opposite direction corresponds to minimum production rate for Q. In the presence of constraints SG-principle suggests that production rate for Q is maximum under imposed constraints. The laws of dynamics under constraints can be found using Lagrange multipliers. The SG-principle applies to a broad class of physical systems subjected to potential and/or dissipative forces, see examples in [6, 10].

SPEED-GRADIENT ENTROPY MAXIMIZATION

Let us underly that the speed-gradient principle provides an answer to the question: **how** the system will evolve? It differs from the principles of maximum entropy, minimum Fisher information, etc. providing and answer to the questions: **where?** and **how far?** Particularly, it means that SG-principle generates equations for the *transient (non-stationary) mode* rather than the equations for the *steady-state mode* of the system. It allows one to study nonequilibrium and nonstationary situations, stability of the transient modes, maximum deviations from the limit mode, etc. Let us illustrate this feature by the example of an entropy maximization problem.

According to the 2nd thermodynamics law and to the Maximum Entropy Principle the entropy of any physical system tends to increase until it achieves its maximum value under constraints imposed by other physical laws. Such a statement provides knowledge about the final distribution of the system states, i.e. about asymptotic behavior of the system when $t \to \infty$. However it does not provide information about the way how the system moves to achieve its limit (steady) state.

In order to provide motion equations for the transient mode, let us employ the SG-principle. Assume for simplicity that the system consists of N identical particles distributed over m cells. Let N_i be the number of particles in the ith cell and the mass conservation law holds:

$$\sum_{i=1}^{m} N_i = N. \tag{6}$$

Assume that the particles can move from one cell to another and we are interested in the system behavior both in the steady-state and in the transient modes. The answer for the steady-state case is given by the Maximum Entropy Principle: if nothing else is known about the system, then its limit behavior will maximize its entropy [4]. Let the entropy of the system be defined as logarithm of the number of possible states:

$$S = \ln \frac{N!}{N_1! \cdot \ldots \cdot N_m!}. \tag{7}$$

If there are no other constraints except normalization condition (6), S is maximized when $N_i^* = N/m$. For large N one may use the Stirling approximation $N_i! \approx (N_i/e)^N$. Then

$$S \approx N \ln \frac{N}{e} - \sum_{i=1}^{m} N_i \ln \frac{N_i}{e} = -\sum_{i=1}^{m} N_i \ln \frac{N_i}{N}$$

which coincides with the standard definition for the entropy $S = -\sum_{i=1}^{m} p_i \ln p_i$, modulo a constant multiplier N, if the probabilities p_i are understood as frequencies N_i/N.

To get an answer for transient mode apply the SG-principle choosing the entropy $S(X) = -\sum_{i=1}^{m} N_i \ln N_i$ as the goal function to be maximized, where $X = \mathrm{col}(N_1, \ldots, N_m)$ is the state vector of the system. Assume for simplicity that the motion is continuous in time and the numbers N_i are changing continuously, i.e. N_i are not necessarily integer (for large N_i it is not a strong restriction). Then the law of motion can be represented in the form

$$\dot{N}_i = u_i,\ i = 1, \ldots, m, \tag{8}$$

where $u_i = u_i(t),\ i = 1, \ldots, m$ are controls – auxiliary functions to be determined. According to the SG-principle one needs to evaluate first the speed of change of the entropy (7) with respect to the system (8), then evaluate the gradient of the speed with respect to the vector of controls u_i considered as frozen parameters and finally define actual controls proportionally to the projection of the speed-gradient to the surface of constraints (6). In our case the goal function is the entropy S and its speed coincides with the entropy production $\dot{S}$. In order to evaluate $\dot{S}$ let us again approximate S from the Stirling formula $N_i! \approx (N_i/e)^N$:

$$\hat{S} = N \ln N - N - \sum_{i=1}^{m} (N_i \ln N_i - N_i) = N \ln N - \sum_{i=1}^{m} N_i \ln N_i. \tag{9}$$

Evaluation of $\dot{\hat{S}}$ yields

$$\dot{\hat{S}} = -\sum_{i=1}^{m} ((u_i \ln N_i + N_i \frac{u_i}{N_i}) = -\sum_{i=1}^{m} u_i (\ln N_i + 1).$$

It follows from (6) that $\sum_{i=1}^{m} u_i = 0$. Hence $\dot{\hat{S}} = -\sum_{i=1}^{m} u_i \ln N_i$. Evaluation of the speed-gradient yields $\frac{\partial \dot{\hat{S}}}{\partial u_i} = -\ln N_i$ and the SG-law $u_i = \gamma(-\ln N_i + \lambda),\ i = 1, \ldots, m$, where Lagrange multiplier λ is chosen in order to fulfill the constraint $\sum_{i=1}^{m} u_i = 0$, i.e. $\lambda = \frac{1}{m} \sum_{i=1}^{m} \ln N_i$. The final form of the system dynamics law is as follows:

$$\dot{N}_i = \frac{\gamma}{m} \sum_{i=1}^{m} \ln N_i - \gamma \ln N_i,\ i = 1, \ldots, m. \tag{10}$$

According to the SG-principle the equation (10) determines transient dynamics of the system. To confirm consistency of the choice (10) let us find the steady-state mode, i.e. evaluate asymptotic behavior of the variables N_i. To this end note that in the steady-state $\dot{N}_i = 0$ and $\sum_{i=1}^{m} \ln N_i = \ln N_i$. Hence all N_i are equal: $N_i = N/m$ which corresponds to the maximum entropy state and agrees with thermodynamics.

Global asymptotic stability of the steady-state mode is proven in [9] by means of the entropy Lyapunov function $V(X) = S_{max} - S(X) \geq 0$, where $S_{max} = N \ln m$. It is seen that $\dot{V} \leq 0$ and the equality $\dot{V}(X) = 0$ holds if and only if all the values N_i are equal, i.e. only at the maximum entropy state. The physical meaning of the law (10) is moving along the direction of the maximum entropy production rate.

Let in addition to the mass conservation law (6) the energy conservation law hold. Let E_i be the energy of the particle in the ith cell and the total energy $E = \sum_{i=1}^{m} N_i E_i$ be conserved. According to the SG-principle one should form the projection of the law (10) onto the surface (in our case – subspace of dimension $m-2$) defined by the relations $\sum_{i=1}^{m} u_i E_i = 0$, $\sum_{i=1}^{m} u_i = 0$. and the evolution law should have the form [9]

$$\frac{d}{dt}\bar{N}(t) = A \ln \bar{N}(t), \tag{11}$$

where symmetric $m \times m$ matrix A is defined as follows:

$$a_{ij} = -\delta_{ij} + \frac{1}{m} + \tilde{E}_i \tilde{E}_j, i, j = 1, \ldots, m$$

$\delta_{ij} = 1$, if $i = j$, $\delta_{ij} = 0$, if $i \neq j$, $\tilde{E}_i = E_i - \frac{1}{m}\sum_{i=1}^{m} E_i$. It depends on the vector of energies $\bar{E} = (E_1, \ldots, E_m)^T$). According to its structure the matrix A is symmetric and has two zero eigenvalues. At the equilibrium point of the system $N_i = C\exp(-\mu E_i)$, $i = 1, \ldots, m$, where $\mu = \lambda_1/\gamma$ and $C = \exp(-\lambda_2/\gamma)$. The value of C can also be chosen from the normalization condition $C = N(\sum_{i=1}^{m} \exp(-\mu E_i))$. We see that equilibrium of the system with conserved energy corresponds to the Gibbs distribution. Again the direction of change of the numbers N_i coincides with the direction of the fastest growth of the local entropy production subject to constraints. As before, it can be shown that $V(X) = S_{max} - S(X)$ is Lyapunov function for the system and that the Gibbs distribution is the only stable equilibrium of the system in non-degenerate cases.

MOLECULAR DYNAMICS STUDY

As an illustration for the above approach we will demonstrate study of the system of interacting particles that are used in modeling physical and mechanical processes by means of particle dynamics [11]. We will consider the simplest system and an approach consistent with the classical molecular dynamics. Such system satisfies the principle of maximum entropy and the required conservation laws (for energy and number of particles) are fulfilled.

A set of particles interacting through the Lennard-Jones potential $\Pi(r)$ is considered.

Initially the particles uniformly fill a cubic volume. Periodic boundary conditions are imposed. The particles inside the volume are initially ordered in a face-centered cubic (FCC) lattice. Step size of the lattice is chosen to ensure a given value of the relative material density $\rho = 0.125$, which is calculated in relation to the close-packed state in which the distance between the nearest atoms is equal to a. To set the initial velocity distribution of the particles we will choose the following law: the velocity vectors are uniformly distributed in the volume of a sphere of radius v_{rand}.

Let T_0 be period of small oscillations of a particle with mass m under the action of an elastic force with the stiffness $C = \Pi''(a)$. The value of T_0 is convenient to take as a microscopic time scale in the system.

For simulation with 256 000 particles the equilibrium distribution density was finally settled at $T = 8T_0$. Qualitatively it corresponds to Maxwell distribution.

The energy area is divided into three intervals:

$$I_1 = \left[0, \tfrac{1}{3}K_{\max}\right), \qquad I_2 = \left[\tfrac{1}{3}K_{\max}, \tfrac{2}{3}K_{\max}\right), \qquad I_3 = \left[\tfrac{2}{3}K_{\max}, +\infty\right). \tag{12}$$

Graph in Fig. 1,a) shows time c
interval I_i, $i = 1,2,3$. Values in t

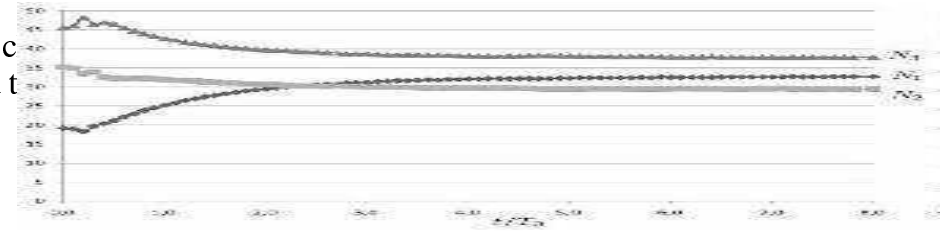

FIGURE 1. a). Dynamics of the populations: $N_1(t)$ (solid line), $N_2(t)$ (dotted line) and $N_3(t)$ (dashed line)/ b). Dynamics of coordinates in the indicative plane.

particles N. The graph shows that for $T = 8T_0$ distribution function tends to the steady state, which is significantly different from the primary. The values of N_i are connected according to identity

$$N_1 + N_2 + N_3 = N, \tag{13}$$

where N is the total number of particles, which remains unchanged. Relation (13) specifies the plane in the space of variables N_1, N_2, N_3 with coordinates $X = \frac{1}{\sqrt{2}}(N_2 - N_1)$, $Y = \frac{1}{\sqrt{6}}(2N_3 - N_2 - N_1)$ called *indicative plane*. Then change of the state of the system will be reflected by movement of the image point on the indicative plane — Fig. 1, b).

STUDY OF SYSTEM EVOLUTION USING SG-METHOD

Let us turn to study of distribution function evolution by entropy SG-method. Let $m = 3$, i.e. particles may take one of three possible states (cells or energy layers)) with energies $E_1 = 0.34, E_2 = 0.83, E_3 = 1.4$, corresponding to average energy in the intervals I_i, $i = 1,2,3$ for uniform distribution, see Fig.2. Let $N_i(t)$, $t \geq 0$ be the number of particles in ith state, $i = 1,2,3$, evolution of $N_i(t)$ obeying mass and energy conservation laws. According to MaxEnt principle the system should tend to the state (N_1^*, N_2^*, N_3^*), that has maximum entropy under two constraints. Let us normalize $N_i(t)$ by total number of particles $N = N_1(t) + N_2(t) + N_3(t)$. Then $N_i(t)$ is a fraction of particles occupying energy level E_i. Denote $E(t) = N_1(t)E_1 + N_2(t)E_2 + N_3(t)E_3$ total energy of the system. Since $N = 1$ total energy coincides with the average energy of a particle $\bar{E}(t) = E(t)/N$.

Let initial distribution of frequencies be: $N_1(0) = 0.367; N_2(0) = 0.023; N_3(0) = 0.61$ and $E = 1$. Numerical integration of (11) shows that in this case the limit state is $N_1^* = 0.213; N_2^* = 0.309; N_3^* = 0.478$, see Fig.2,a.

In the indicative plane we have $X(t) \to X^*, Y(t) \to Y^*$ as $t \to \infty$, where $X^* = -0.068, Y^* = 0.1767$. As seen from Fig.2,b, the solution belongs to the plane inclined with the slope $K = \Delta Y / \Delta X \approx 0.52$. It is easy to see that convergence to the limit distribution is exponential.

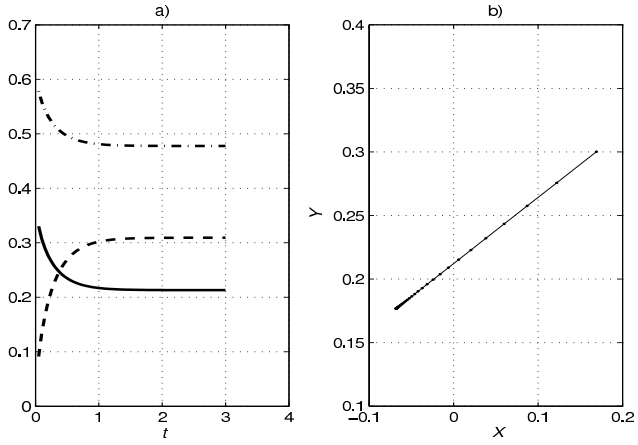

FIGURE 2. a). Dynamics of the populations: $N_1(t)$ (solid line), $N_2(t)$ (dotted line) and $N_3(t)$ (dashed line)/ b). Dynamics of coordinates in the indicative plane.

DISCUSSION

Calculations with different numbers of particles show that, while smoothness of the graphs is increasing with increasing number of particles the main tendencies are the same. Fast transient processes with significant changes of distribution function take place for $t < T_0$. After that a slow evolution of the distribution function takes place until $t = 4T_0$. The final distribution agrees with Maxwellian one and does not depend on initial one. Trajectory of image point in the indicative plane visualizes change of the distribution function. For $t > T_0$ image point trajectory becomes almost a straight line that coincides with the prediction based on entropy SG-principle.

Comparison with the results based on entropy SG-principle for the case of three energy cells clearly shows coincidence of the main tendencies: the system reaches a stationary distribution not depending on initial one; after fast transients it approaches stationary distribution along the straight line. Numerical comparison is given the table 1. The numbers N_i^* are normalized by the total number of particles N. It can be seen

TABLE 1. Comparison of results obtained by the two methods.

Method	N_1^*	N_2^*	N_3^*	X^*	Y^*	$\Delta Y/\Delta X$
SG-principle	0.213	0.309	0.478	-0.068	0.1767	0.52
Particle dynamics	0.33	0.29	0.38	-0.024	0.055	0.67÷0.78

that the values N_i^*, obtained by two methods are close. The difference in the values of the slope $\Delta Y/\Delta X$ is $20\% - 30\%$. The values of the slope obtained by the molecular dynamics method based on spherical and globular initial velocity distributions differ not significantly. The errors are within the computation precision.

Therefore simulation results for a complex system with a large number of degrees of freedom agree with the results for a low number of DOF based on SG-principle. It underlines the benefits of the SG-method for qualitative analysis of systems of particles and molecular dynamics.

CONCLUSIONS

Speed-gradient variational principle provides a simple yet useful addition to classical results in thermodynamics. Whereas the classical results allow researchers to answer the question "Where it tends to?", the speed-gradient approach provides an answer to the question: "How it reaches its steady-state mode?". If entropy is chosen as the goal function then the SG-principle complements the Gibbs-Jaynes MaxEnt principle and allows one to find the direction of the trend to the MaxEnt state. In other words, if the Nature tends to a 'maximally unknown' state, then it does it with maximum speed.

The results of this paper provide, on the one hand, numerical evidences of the SG-principle. On the other hand, the results demonstrate applicability of the SG-principle to the predictions of systems of particles and molecular dynamics.

ACKNOWLEDGMENTS

The work was supported by Russian Foundation for Basic Research (project RFBR 08-01-00775, 08-01-00865, 09-01-12096-ofi-m) and Research Program 02 of OEMMPU Division of RAS. The authors like to thank Ilya Izrailevich Blekhman for continuous moral support of their works.

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