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Research, Education and Industry Linkage*

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Editors: W.Y.D. Yuen, P. Broadbridge, J.M. Steiner



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Nonconservation Law Equation In Mathematical Modelling: Aspects Of Approximation

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Abstract. In this paper we treat mathematical and computational models of thermodynamical systems in viscous and diffusive media as optimal information control problems. Under assumption of sufficient smoothness on the perturbed Hamiltonian of the system we propose reformulations of the classical problems using the concept of informational limit. In the general situation we use Steklov's operator technique to derive generalisations of classical Hamilton-Jacobi-Bellman (HJB) equation in stochastic, nonsmooth and deterministic cases. We show that nonconservation law equation appears in a natural way from such a consideration. For its approximation we use an evolution-associated Markov Chain which permits us to derive stability conditions for our computational model. Computational models of this type give a description of generalised dynamical systems (GDS) which include the modeler (decision maker \equiv DM) as an intrinsic part.

Associated problems of mathematical modelling in semiconductor technology (including modelling of multilayered structures and superlattices) are discussed.

1. Macroscopic thermodynamical systems and non-conservation law.

Many challenging mathematical problems with a wide range of engineering applications arise from the coupled field theory where interconnection of at least two physical (chemical or biological) fields is essential to obtain a plausible picture of phenomena, processes etc.

Presence of a hyperbolic-type operator in many mathematical models of the coupled field theory precludes an assumption (often made *a priori*) that subgrid (microscopic) phenomena can be extracted from macroscopic flow (see Oran and Boris [1]). On the other hand approaches based on a parabolisation of the model and attempts to solve the problem of coherent feedback of small scales with respect to large ones by adding a smoothing diffusion-type term into the model in many cases are not adequate to the physics of the process.

The mathematical and computational problems which arise from the coupled field theory (dynamical thermoelasticity, piezoelectricity and semiconductor device modelling, Melnik [2-4]) was the original stimulation for this paper in which we revise the concepts of deterministic mathematical models and conservation law in mathematical modelling.

As a rule rigorous mathematical justifications of dynamical system evolution is based on an *a priori* assumption of system conservativeness and/or ergodicity. Whereas the first assumption has its roots in Newton-Hamilton classical mechanics, the second one is grounded on the never-proved Gibbs conjecture (Goldstein [5]). Formally a division between Hamiltonian and ergodic systems can be seen as a division between the following two classes of mathematical models:

- models which are "more hyperbolic than non-linear";
- models which are "more non-linear than hyperbolic".

There are many mathematical models which have features of both classes. Among them mathematical models in semiconductor device technology. Mathematical models of semiconductor device simulation usually includes two interconnected parts originated from the Boltzmann kinetic equation and the Maxwell system for electromagnetic field. Though both parts are always subject to approximation in its essence the situation is not different from that arising from classical Newton-Hamilton mechanics. In fact, in addition to the equation(s) of motion (or transport equation) we always have "the law of acting forces" (the second Newton law, Maxwell's system or Poisson's equation etc.), i.e. the equation(s) which define the Hamiltonian of the system (using in general the distribution function $f(x, v, t)$).

Adequacy of the solution of Boltzmann's equation is predetermined by the adequacy of an approximation of the gravitational part of the energy of such a dynamical system, i.e. by "the law of acting forces". In the general case the inverse statement is again true which enables us to talk about the solution only as a pair of functions. In fact, we study the system evolution in Boltzmann's phase space (x, v) , using a mathematical model as an appropriate (for engineering purposes) approximation.

The limiting case of such situations is the scalar conservation law which is considered in spacetime (x, t) . It has a unique generalised solution from L^∞ provided we add to such a mathematical model (which consists of one equation) an additional equation of entropy condition. Computational models in this case are based on the monotone approximating schemes with convergence only in L^1 -norm of configurational space (Crandall and Majda [6]).

Considerations of single-equation-based mathematical models are connected with an assumption that information (with infinite precision) about the gravitational part of the system energy together with the initial density of the system might be provided. In this case we come to the Liouville equation (continuity of probability density) in the Gibbs phase space. The validity of this conservation law (which cannot be justified within the framework of Hamiltonian systems) is based on the Gibbs conjecture which asserts that the appropriate description of a macroscopic system in thermodynamic equilibrium is provided by certain probability measures on the (Gibbs) phase space of the system. The corresponding probability measure should possess the stability property (Goldstein [5]). However stationarity and absolute continuity properties of such probability measures (related to ergodicity assumption) are far from obvious. A balance between drift and diffusion (under the assumption that points of the Gibbs phase space in initial conditions for differential equations can be determined with infinite precision) cannot be found adequately after the passage to the Fokker-Planck equation. The latter can define (approximate) the evolution-associated Markov Chain transition probabilities only on the short time interval (see, for example, Honerkamp [7]). On the one hand such an equation is not conservative *a priori* because of the inevitable loss of some information under its derivation. On the other hand ergodicity assumption might be imposed only if preservation of measure stability is guaranteed.

To approach the problem of dynamics on big (space)time scales we usually pass to the first few moments in Boltzmann's equation obtaining hydrodynamic-type models in configurational spaces. It is a well-known fact that this approach is also connected with the loss of some additional information about the system. The amount of information lost by such a transition and by an approximation of the gravitational part of energy (for example, by the Poisson equation) have to be controlled. However to assert that the conservation energy law is satisfied *a priori* in dynamical systems described by such models is not appropriate.

Optimal information control in mathematical models of dynamical systems is based on the fact that the density alone cannot define evolution of any thermodynamical system. Density is always adapted to the characteristics of the medium where evolution takes place. The latter means stability of such dynamical systems.

2. Informational limit and generalised energy equations of the HJB-type.

Let a dynamical system evolution be described by the idealised mathematical model:

$$H_0^0(t, x, p) = 0, \quad (2.1)$$

where H_0^0 and p denote some mathematical objects (for example, function or functional, space-time derivative or vector field). Since we do not know the precise Hamiltonian of the system we use another mathematical model:

$$H_{\epsilon(\delta)}(t, x, p) = \epsilon(\delta), \quad (2.2)$$

where $H_{\epsilon(\delta)}$ is a perturbed Hamiltonian-related mathematical object (function or functional).

To conduct mathematical reasoning we assume that abstract model (2.1) is true and impose on the perturbed mathematical object (for example, Hamiltonian or velocity function) some *a priori* regularity

assumptions to obtain the result in a lower dimensional space (usually for trajectory $x(t)$ or density). Under such reasoning we do not take into account that dimensionalities of these spaces are selfconsistent and are subject to stability of dynamical system described by the perturbed model (2.2). This is equally true for such equations as the equation $\frac{dx}{dt} = v(t, x)$, stochastic differential equations, Liouville's equation, the Fokker-Planck equation as well as for classical HJB equation, which, in fact, can be considered as special cases of the model (2.2).

Moreover models (2.1) and (2.2) should have consistent regularities. To put it in a different way the validity of the perturbed models depends on the validity of the idealised model and they should be consistent in the the informational limit $\epsilon(\delta) \rightarrow 0$. The latter means that it is more reasonable to consider instead of (2.2) the following extended mathematical model:

$$\lim_{\epsilon(\delta) \rightarrow 0} H_{\epsilon(\delta)}(t, x, p) = 0, \quad \lim_{\epsilon(\delta) \rightarrow 0} D_L H_{\epsilon(\delta)}(t, x, p) = 0, \quad (2.3)$$

where D_L denote the Lie derivative by virtue of the perturbed system (which is characterised by the perturbed velocity v_ϵ or by the perturbed Hamiltonian H_ϵ and the level of perturbations).

However for the generalised model (2.3) where the stability issue is taken into account Hausdorff topology spaces appear to be inappropriate to guarantee the measure stability in the computational sense. On the other hand though computational models for (2.2) are well-established the associated solution of the model (2.2) is not obligatory better of L^1 -function in a configurational space (see Rosovskii [8], Melnik [9]). Even imposing formally excessive a priori smoothness assumptions on the solution of mathematical model (2.2) we return to the stability problem for dynamical systems on the computational level. At the same time the stability issue is automatically included into the generalised mathematical model (2.3).

Therefore, we have three interconnected problems related to the topology of Boltzmann's phase space, the measure stability of the (non-Hausdorff) Gibbs phase space, and the stability of the associated computational models in the configurational space.

The rest of the paper is organised in order to put forward the idea of looking at the mathematical models as an object of optimal information control. Hence, in the rest of this section we give the mathematical background of such a consideration. In section 3 we consider some physical and engineering features of mathematical models using examples from microelectronics. In the concluding section we sketch out the main ideas with respect to the associated computational models.

The close connection of classical Bellman's results in optimal control theory with the Markovian character of evolution is well-known (Sukharev [10]). Attempts to generalise these ideas to the continuous case lead to the viscosity solution theory. It reveals the close connection between nonlinear PDE and optimal control problems (Lions [11], Fleming and Soner [12]). However derivation of the classical HJB equation was conducted under *a priori* smoothness assumption on the unknown function. We have used Steklov's operator technique to relax such assumptions using the local optimality principle (Melnik [9]).

Let us consider the following stochastic optimal control problem (see, for example, Kushner and Dupuis [18]):

$$E_{x,t}^u[J(u)] \rightarrow \min, \quad x(t) = x(t_0) + \int_{t_0}^t f(\tau, x(\tau), u(\tau)) d\tau + \sigma(s, x(s), u(s)) d\omega(s), \quad u \in U, \quad (2.4)$$

where

$$J(u) = \int_{t_0}^T f_0(\tau, x(\tau), u(\tau)) d\tau \rightarrow \min \quad (2.5)$$

(for the Mayer's problem or with the addition term of $g(T, x(T))$ for the Boltz problem). Then the following result gives the connection between optimal control mathematical models (2.4), (2.5) and nonlinear PDEs under relaxed smoothness assumptions.

Theorem 2.1. *The stochastic optimal control problem (2.4), (2.5) can be reduced to the following generalised energy equation:*

$$Lu \equiv (1 + v)[\frac{\partial u}{\partial x} + \frac{1}{v}(\frac{\partial u}{\partial t} + f_0)] + \omega_1 \frac{\partial^2 u}{\partial t \partial x} + \omega_2 \frac{\partial^2 u}{\partial x \partial t} - \sigma_1 \frac{\partial^2 u}{\partial x^2} - \sigma_2 \frac{\partial^2 u}{\partial t^2} = 0 \quad (2.6)$$

with respect to the uncertainty pressure function induced by the control (here $v = \frac{\omega_1}{\omega_2}$, $\sigma_i = \sigma_i(t, x, \omega_1, \omega_2)$, $\omega_i \neq 0$, $i = 1, 2$). The solution is understood as a function from $W_1^{1,1}(Q)$ in the generalised sense as the following integral equality:

$$\int \int_Q S^x \otimes S^t L u \chi_Q(x, t) dx dt = 0 \quad (2.7)$$

If $f_0, g, f \in L^1(Q)$ and $F = f_0(1 + \frac{1}{v}) \in L^1_{Lip}(Q)$, $Q = \{(x', t') : x \leq x' \leq x + \Delta x, t \leq t' \leq t + \Delta t\}$ then there exists a unique generalised solution of (2.6). If $u(t, x) \in W_1^{2,2}(Q)$ it has the second and mixed generalised derivatives.

Here S^t and S^x are Steklov operators (see, for example, Melnik [2]).

In the nonsmooth deterministic case:

$$J(u) \rightarrow \min, \quad \frac{dx}{dt} = f(t, x, u) \quad a.e. \quad \text{in } [t_0, T], \quad x(t_0) = x_0, \quad u \in U \quad (2.8)$$

we obtain the first order approximation $O(\Delta t + \Delta x)$ of the local optimality principle, which is formally the equation (2.6) when $\sigma_1 = \sigma_2 = 0$. The theorem analogous to 2.1 was proved.

The deterministic limit of optimal control theory leads to the following result.

Theorem 2.2. If $u(t, x) \in L^1(Q)$ the optimal control problem (2.8) can be reduced to the following generalised energy equation:

$$Lu \equiv (1+v)[\frac{\partial u}{\partial x} + \frac{1}{v}(\frac{\partial u}{\partial t} + f_0)] = 0. \quad (2.9)$$

The solution is understood in the generalised sense of the integral equality (2.7). If $f_0, g, f \in L^1(Q)$ and F satisfies the locally relaxed Lipschitz condition:

$$\|S^x \otimes S^t[F(t, x, u') - F(t, x, u'')] \|_{L^1(Q)} \leq q \|S^x \otimes S^t[u' - u'']\|_{L^1(Q)}$$

then there exists a unique generalised solution of (2.9).

The proof of this theorem is constructive and based on the use of Feer's sums.

Let us introduce two vector fields $\vec{\psi} = (\psi_1, \psi_2)$ and $\vec{H} = (H_1, H_2)$, where

$$\psi_1(t, x) = \int_x^{x+\Delta x} u(\mu, t) d\mu, \quad \psi_2(t, x) = \int_t^{t+\Delta t} u(x, \eta) d\eta \quad (2.10)$$

$$H_1 = S^t \otimes S^x \int_t^{t+\Delta t} f_0 d\tau + S^t \psi_1, \quad H_2 = S^x \otimes S^t \int_t^{t+\Delta t} f_0 d\tau + S^x \psi_2. \quad (2.11)$$

Then for the nonsmooth case we have:

Theorem 2.3. If $\omega_1 + \omega_2 = 2$ then in Q we have the following equality to be understood in the almost everywhere sense:

$$\frac{\partial H_1}{\partial t} \frac{\partial H_2}{\partial x} = (\operatorname{div} \vec{\psi})^2.$$

Under corresponding smoothness assumptions for the point of local optimum:

$$\operatorname{div} \vec{\psi} = \operatorname{div} \vec{H} = 0, \quad \frac{\partial^2 H_1}{\partial t \partial x} = \frac{\partial^2 H_2}{\partial x \partial t}. \quad (2.12)$$

In the general case we have

Theorem 2.4. The Lie derivative of the Hamiltonian vector field (2.11) (i.e. the derivative in the direction of the vector field of solution (2.10)) is equal to zero. For the local optimum point (2.12) is true under the corresponding smoothness assumptions.

This result, obtained for stochastic optimal control problems, is in agreement with the mathematical model (2.3) in informational limit. Associated with this limit computational models are related to the deterministic limit of the optimal control theory. They are the subject of our consideration in section 4.

Now as an example of mathematical models of thermodynamic systems in viscous and diffusive media we turn our attention to mathematical models of semiconductor devices.

3. Semiconductor technology and mathematical modelling.

One of the most challenging area of mathematical model applications is microelectronics. Nonlocal and nonequilibrium features of the dynamics of semiconductor plasma imply a close cooperation between mathematicians, physicists and engineers.

Due to the achievements of semiconductor technology it is now possible to create multilayered structures, among which are semiconductors with superlattices (SWS). Such semiconductors as well as many other devices of acoustoelectronics have far reaching engineering applications (see Bass et al [13], Melnik [14]). In

electromagnetic fields such structures become active with the development of different kinds of instabilities which can be used in many technical devices. Moreover in some cases (for example, quantum superlattices) this is true even under low levels of signal.

Though the computational physics of semiconductor technology has been developing quite rapidly and successfully, for many problems in semiconductor device analysis mathematicians approach this field of investigation very cautiously. This fact is not surprising if we take into consideration that mathematically-convenient superposition principles do not work here and non-linear parts of corresponding operators cannot be treated as some perturbation. In semiconductor physics nonlinear terms are not only important but as a rule dominant. If in addition we recall normalisation problems with respect to computational models we can easily explain the cautious approach of mathematicians in this field.

Many mathematically challenging problems can be seen even in the example of relatively simple drift-diffusion model for semiconductor devices. This includes, for example, Tamm levels and high-level-doping effects which, in fact, are prototypes of surface waves in superlattices. Now it is obvious that for the GaAs technology such drift-diffusion models are not adequate for engineering design purposes. The hydrodynamic type of models manifests the next step in the semiconductor device simulation. However including into models the conservation energy law leads to serious mathematical difficulties related to the stability of constructed computational models (Melnik [15]). In multilayered structures this problem becomes even more difficult.

Can mathematical models in semiconductor device technology be considered in the form of deterministic systems of PDEs? Or is it rather a subject of optimal information control theory? Below we give some engineering and physical reasons why we believe in the second approach which implies presence of a modeler (DM) as an intrinsic part of the model itself.

- Even for classical drift-diffusion models for semiconductor devices evaluation of mobility is always a subject to the solution of an optimisation problem with respect to certain parameters which we pick up from experiments. In fact, this is a part of the much more general problem of the connection between mobility and diffusion coefficients for all mathematical models in semiconductor device theory. The solution of this important and challenging problem leads to an inevitable approximation of the gravitational part of system energy and as a result to an inevitable approximation of conservation laws. The adequacy of such approximations is to be determined by the modeler.
- It is a well-known fact that high levels of doping make it necessary to study zone structures of semiconductors (see Mulyarchik [16] and references therein). Attempts to establish "tails" of state densities in the forbidden zone can be made only on the basis of Fermi-Dirak statistics rather than Boltzmann. The main problem of such an approach is in *an adequate measurement of "the effective width of forbidden zone contraction"* (EW). However the other approach is to consider EW as a parameter of adjustment between computed and measured output characteristics of our structure (Mulyarchik [16], Polsky and Rimshans [17]). Though in this way we can avoid the engineering problem of EW measurement, EW as a function should be included into the definition of the problem generalised solution.
- A similar situation arises for SWS (Bass et al [13]). In fact, we use advantages of nonhomogeneous media in comparison with homogeneous media (not simply appreciate the fact of their existence). Interactions between optic and acoustic waves can be controlled using the evaluation of the threshold for the forced Mandelshtam-Brillouin dispersion (defined by fading coefficients for acoustic and optic signals and the nonlinear function of their connection).

In general we can say that the success of modelling depends not only on the mathematical model itself but on the control of the modeler. The latter can be conducted by the adaptive choice of medium (doping or material) and the topology of such medium. Since we use nonuniform (position-dependent) band structure of medium, the mathematical solution of such problems can be formalised only as pairs of functions which relate densities to characteristics of the medium. Hence, even if we assume that characteristic lengths of the structure exceed fundamental characteristic lengths (such as Debye radius), the waves in such structures gain a "quantum character" and densities do not have to be continuous functions.

4. Computational models as Markov Decision Processes.

The majority of mathematical models (both deterministic and stochastic) treat time as a deterministic category (a small number of exceptions are related to Landau decay effects). However, if we assume that the dynamical system is controlled, such a consideration seems to be inappropriate in general. Such control

as a function is subject to the intrinsic uncertainty in the mathematical model itself. As a result the model itself should be correlated with this uncertainty. Therefore the problem of mathematical modelling is to estimate such uncertainty using the sequential character of evolution rather than to eliminate it from the mathematical model by some kind of smoothing procedures.

The appropriate basis for such estimation gives the nonconservation law equation which can be obtained from the deterministic limit of optimal control theory (2.9) when $f_0 = 0$:

$$\frac{\partial u}{\partial t} + v_{macro}(t, x, u) \frac{\partial u}{\partial x} = 0, \quad (4.1)$$

where v_{macro} is a control-adapted approximation to the real velocity of the system. The modeler (DM) is included into the model by the specification of the (macro)velocity of the system (as an approximation of the real velocity) and by the identification of two macroscopic (with respect to his (space)time) events. Then we consider the mathematical model which consists of two equations: nonconservation law with respect to uncertainty pressure (control) and genuine microscopic dynamics of the system itself $\frac{dh}{d\tau} = v_{micro}(\tau, h, u)$, where v_{micro} is an approximation of the microcomponent of the real velocity function of the system. Both parts of the perturbed velocity function (which are constituents of an approximation to the real velocity) inherit their dependency on the uncertainty pressure (control) function. Systems described by such coupled equations we call generalised dynamical systems (GDS). The solution pair $(h(\tau), u(t, x))$ of such mathematical model defines a Markov process, which we propose to approximate by the evolution-associated Markov Chain (see references in Kushner and Dupuis [18]).

Definition 4.1. A Markov Chain $\xi_n^{\tau h}$, $n < \infty$ is consistent with the Markov process $(h(\tau), u(t, x))$ defined by the mathematical model of GDS evolution if the following equalities hold:

$$E_n^{\tau h|(x_i, u^j)} \Delta \xi_j^{\tau h} = v_{macro}(x_i, t^j, u^j) \tau + o(h + \tau). \quad (4.2)$$

$$cov_n^{\tau h|(x_i, u^j)} \Delta \xi_j^{\tau h} = o(h + \tau). \quad (4.3)$$

We refer to the condition (4.2) as the condition of local consistency whereas to (4.3) as the global consistency condition.

Remark 4.1. The equalities (4.2), (4.3) imply the following fact: the macroscopic properties of the system should not change dramatically in small (with respect to the whole evolution) DM-time-interval, though microscopic properties can vary significantly subject to the velocity function. Another way of putting it is that consistency conditions referring to the probabilistic microscopic level make explicit basic features of system evolution on the macroscopic level. The same role in physics plays the second law of thermodynamics (Misra and Prigogine [19]). We proved the following theorem on the Markov Chain approximation stability.

Theorem 4.1. If transition probabilities of a Markov Chain $(\xi_n^{\tau h}, n < \infty)$ are defined by the formulae:

$$p^{\tau h}[x_k^j, x_i^{j+1} | d(x_k^j, t^j)] = \begin{cases} 1 - \frac{\tau}{h}(|v| + v^- \gamma_4 - v^+ \gamma_1) & k = i \\ \frac{\tau}{h}[v^+(1 + \gamma_2) + v^- \gamma_4] & k = i - 1 \\ \frac{\tau}{h}[v^-(1 - \gamma_3) - v^+ \gamma_1] & k = i + 1 \\ -\frac{\tau}{h}(v^+ \gamma_2) & k = i - 2 \\ \frac{\tau}{h}(v^- \gamma_3) & k = i + 2 \\ 0 & \text{otherwise} \end{cases}$$

$\forall j = \overline{0, n-1}$ and $i = \overline{j, N-j}$ ($\gamma_2 = 0$ for $i = j$ and $\gamma_3 = 0$ for $i = N-j$) whereas the interpolation interval τ satisfies the conditions

$$1 - \frac{\tau}{h}(|v| + v^- \gamma_4 - v^+ \gamma_1) \geq 0, \quad \gamma_2 \leq 0, \quad \gamma_3 \geq 0, \quad (4.4)$$

$$v^+(1 + \gamma_2) + v^- \gamma_4 \geq 0, \quad v^-(\gamma_3 - 1) + v^+ \gamma_1 \leq 0. \quad (4.5)$$

$$\frac{\tau}{h} \leq \frac{v^+(1 - \gamma_1 - 3\gamma_2) + v^-(1 + \gamma_4 + 3\gamma_3)}{[v^-(1 + \gamma_3 - \gamma_4) - v^+(1 + \gamma_1 - \gamma_2)]^2} \quad (4.6)$$

then the Markov Chain approximation of the process $(h(\tau), u(t, x))$ is stable and discrete values of the uncertainty pressure (DM-function) can be found from the following formula:

$$d(x_i^{j+1}, t^{j+1}) = \sum_k p^{\tau h}[x_k^j, x_i^{j+1} | d(x_k^j, t^j)] d(x_k^j, t^j). \quad (4.7)$$

Here $v^+ = \max[v, 0]$, $v^- = \max[-v, 0]$ (index macro is omitted for simplicity) and γ_i , $i = \overline{1, 4}$ are flux limiters defined for upwind approximation.

Remark 4.2. When $n \rightarrow \infty$ the velocity of the Markov Chain converges to the velocity of the process in a sense of the Markov theorem on the generalised law of big numbers.

In general we have the whole family of discrete Markov decision processes (DMDP) defined as follows

$$\mathcal{M}(e_0, e_1, \dots, e_{n_0}) = \{\mathcal{D}(i; j), R(e_j \rightarrow e_{j+1}), p_j^{j+1}(k; i), i = \overline{n_j, N_j}, j = \overline{0, n_0}\}, \quad (4.8)$$

where $p_j^{j+1}(k; i) = p^{h\tau}[x_k^j, x_i^{j+1} | d(x_k^j, t^j)]$; $\mathcal{D}(i; j) = \Xi(i; j) \times \mathcal{A}(i; j)$ (allowable decision set for each macroscopic event e_j , $j = \overline{0, n_0}$); $\mathcal{A}(i; j) = \{d(t^j, x_i^j), i = \overline{n_j, N_j}\}$ (action set); $\Xi(i; j) = \{x_i^j, i = \overline{n_j, N_j}\}$ (cone of macroscopic events with probabilistic model for each of them as $e_j \equiv \{\mathcal{D}(i; j); p_i^j\}$); and $R(e_j \rightarrow e_{j+1}) = (\{(x_i^{j+1}, d(t^{j+1}, x_i^{j+1}); p_i^{j+1}\}, i = \overline{n_{j+1}, N_{j+1}})$ (reward set); $n_0 = n_0(T, t_0, h(\tau))$ (a finite number of observed macroscopic events). Each of such a DMDP constructs a **probabilistic trajectory of system evolution**:

$$T(k_0, \dots, k_{n_0}) = \{p_0^0(k_0), p_0^1(k_0; k_1), p_1^2(k_1; k_2), \dots, p_{n_0-1}^{n_0}(k_{n_0-1}; k_{n_0})\},$$

($k_l \in [n_l, N_l]$, $l = \overline{0, n_0}$) in the cone of macroscopic events. In general the equality $p_{n_0-1}^{n_0}(k_{n_0-1}; k_{n_0}) = 1$ cannot be guaranteed and a closeness of this probability to 1 depends on values of $p_0(k_0)$ and the structure of the cone of macroscopic events (i.e. on the approximation of e_0 and e_{n_0}).

The optimal probabilistic trajectory is defined by the optimal Markov policy which corresponds to the construction of such a Markov Chain which evolves to the most probable state of the system preserving the property of strong causality of macroscopic events.

From the computational point of view such a policy has much in common with numerical procedures related to the coupled diffusion-dispersion (CDD) phenomenon. This phenomenon is often connected with the presence of regions with big gradients which is typical, for example, for semiconductor device modelling. We also admit a connection on the computational level between nonsmooth deterministic and stochastic optimal control problems discussed in section 2. Such a connection seems to be intrinsic for the class of generalised solutions from $W_1^{1,1}(Q)$. Amongst computational procedures of this type we admit nonlinear monotone difference schemes and, in particular, FCT method (Oran and Boris [1], Melnik [4]). At present discontinuous weighting functions are widely used in FEM (Aluru et al [20]) and admissibility of discontinuous basis functions in BEM is seen as an advantage (Lee and Palisoc [21]). A measure of the adequacy of results of mathematical modelling to the real evolution of dynamical systems can be effectively defined with respect to the presence of the modeler which is included in mathematical (and computational) models by allowing for discontinuous solutions.

5. Conclusions and Future Directions.

We have considered mathematical models where microscopic subgrid phenomena influence the macroscopic properties of the system yet the former cannot be extracted from the latter. A unified approach for such system descriptions has been proposed on the basis of evolution-associated Markov Chains.

Global inseparability of the velocity function from medium perturbations implies a stabilization procedure for any mathematical model we use. Such procedure is based on an evaluation of uncertainty pressure and has physical roots in inevitable approximation of the gravitational part of system energy. The key equation for such evaluation is the nonconservation law equation which is a part of the general GDS model. The intrinsic connection of GDS with optimal control theory has been emphasised and some generalisations in this field have been obtained. The area of applications of nonconservation law equations is rapidly expanding in engineering, physics, chemistry and biology. As an example we have discussed mathematical models of semiconductor analysis which we look at as problems of optimal information control. The latter forces us once again to rediscover the importance of the second law of thermodynamics, which makes explicit on the macroscopic level a basic structure referring to the microscopic level. It gives us a way to control instability of dynamical systems which being nonuniform themselves evolve in nonuniform perturbative media.

Further development of semiconductor technology on the basis of multilayered structures such as superlattices is closely connected with adequate representation in physical and mathematical models of thermal and magnetic fields subject to approximation in computational models (Kalnibolotsky et al [22]).

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