Chaos in N-body problem.

Michail Zak
Senior Research Scientist (Emeritus)
Jet Propulsion Laboratory California Institute of Technology
Pasadena, CA 91109

Abstract.

1. Introduction.

The ***n*-body problem** is the problem of predicting the individual motions of a group of objects interacting with each other via conservative forces. These forces can be of gravitational origin (celestial mechanics), inter-molecular origin (molecular dynamics), or representing the Coulomb potential (structural biology). In the most common version, the trajectories of the objects are determined by numerically solving the Newton's equations of motion for a system of interacting particles. Non-conservative version of the interaction forces became important in case of the *n*-body problem that incorporates the effects of radiation pressure, Poynting-Robertson (P-R) drag, and solar wind drag.

The *n*-body problem as a classic astronomical and physical problem that naturally follows from the two-body problem first solved by Newton in his *Principia* in 1687. The efforts of many famous mathematicians have been devoted to this difficult problem, including Euler and Lagrange (1772), Jacobi (1836), Hill (1878), Poincaré (1899), Levi-Civita (1905), and Birkhoff (1915). However, despite centuries of exploration, there is no clear structure of the solution of the general *n*- or even three-body problem as there are no coordinate transformations that can simplify the problem, and there are more and more evidences that, in general, the solutions of *n*-body problems are chaotic. Failure to find a general analytical structure of the solution shifted the effort towards numerical methods. Many ODE solvers offer a variety of advance numerical methods for the solution. The general method of numerical solution of the corresponding system of ODE was originally conceived within theoretical physics in the late 1950s,[1,2], but is applied today mostly in chemical physics, materials science and the modeling of biomolecules.

The most significant "side effect "of the existing numerical methods for n-body problems becomes chaos when different numerical runs with the same initial conditions result in different trajectories. Although numerical errors can contribute to chaos, nevertheless the primary origin of chaos is physical instability, [3].

In this work, a general approach to probabilistic description of chaos in n-body problem with conservative and non-conservative interaction forces is proposed.

2. Chaos in classical dynamics

We start this section with revisiting mathematical formalism of chaos in a non-traditional way that is based upon the concept of orbital instability.

The concept of randomness entered Newtonian dynamics almost a century ago: in 1926, Synge, J. introduced a new type of instability - orbital instability- in classical mechanics, [4], that can be considered as a precursor of chaos formulated a couple of decades later, [5]. The theory of chaos was inspired by the fact that in recent years, in many different domains of science (physics, chemistry, biology, engineering), systems with a similar strange behavior were frequently encountered displaying irregular and unpredictable behavior called chaotic. Currently the theory of chaos that describes such systems is well established. However there are still two unsolved problem remain: prediction of chaos (without numerical runs), and analytical description of chaos in term of the probability density that would formally follow from the original ODE. This paper proposes a contribution to the solution of these problems illustrated by chaos in inertial systems

a. Orbital instability as a precursor of chaos.

Chaos is a special type of instability when the system does not have an alternative stable state and displays an irregular aperiodic motion. Obviously this kind of instability can be associated only with ignorable variables, i.e. with such variables that do not contribute into energy of the system. In order to demonstrate this kind of instability, consider an inertial motion of a particle M of unit mass on a smooth pseudosphere S having a constant negative curvature G_0, Fig. 1.

$$G_0 = const > 0 \qquad (1)$$

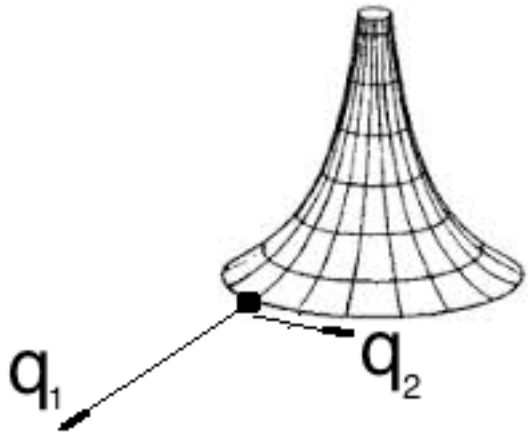


Figure 1. Inertial motion on a smooth pseudosphere.

Remembering that trajectories of inertial motions must be geodesics on *S*, compare two different trajectories assuming that initially they are parallel, and the distance ε_0 between them, is small (but not infinitesimal!),

$$0 < \varepsilon_0 << 1 \qquad (2)$$

As shown in differential geometry, the distance between these geodesics increases exponentially

$$\varepsilon = \varepsilon_0 e^{\sqrt{-G_0}q_1}, \quad G_0 < 0, \qquad (3)$$

Hence no matter how small the initial distance ε_0, the current distance ε tends to infinity as q_1 increases.

Let us assume now that accuracy to which the initial conditions are known is characterized by the scale *L*. This means that any two trajectories cannot be distinguished if the distance between them is less than *L* i.e. if

$$\varepsilon < L \qquad (4)$$

The period during which the inequality (4) holds has the order

$$\Delta t \approx \frac{1}{\sqrt{|-G_0|}} \ln \frac{L}{\varepsilon_0} \qquad (5)$$

However for

$$t >> \Delta t \qquad (6)$$

these two trajectories diverge such that they can be easily distinguished and must be considered as two different trajectories. Moreover the distance between them tends to infinity no matter how small is ε_0. That is why the motion once recorded cannot be reproduced again (unless the initial condition are known exactly), and consequently it attains stochastic features. The Liapunov exponent for this motion is positive and constant

$$\sigma = \lim_{\substack{t\to\infty \\ \varepsilon_0\to 0}} [\frac{1}{t}\ln\frac{\varepsilon_0 e^{\sqrt{-G_0}t}}{\varepsilon_0}] = \sqrt{-G_0} = const > 0 \qquad (7)$$

Remark. In theory of chaos, the Liapunov exponent measures divergence of initially close trajectories averaged over infinite period of time. But in this particular case, even "instantaneous" Liapunov exponent taken at a fixed time has the same value (7).

Let us introduce a system of coordinates on the surface *S*: the coordinate q_1 along the geodesic meridians and the coordinate q_2 along the parallels. In differential geometry such a system is called semigeodesic. The square distance between adjacent points on the pseudosphere is

$$ds = g_{11}dq_1^2 + 2q_{12}dq_1dq_2 + g_{22}dq_2^2 \qquad (8)$$

where

$$g_{11} = 1, \quad q_{12} = 0, \quad g_{22} = -\frac{1}{G_0}e^{(-2\sqrt{-G_0}q_1)} \qquad (9)$$

The Lagrangian for the inertial motion of the particle *M* on the pseudosphere is expressed via the coordinates and their temporal derivatives as

$$L = g_{ij}\dot{q}_i\dot{q}_j = \dot{q}_1^2 - \frac{1}{G_0}e^{(-2\sqrt{-G_0}q_1)}\dot{q}_2^2 \qquad (10)$$

and consequently,

$$\frac{\partial L}{\partial q_2} = 0 \qquad (11)$$

$$\frac{\partial L}{\partial q_1} \neq 0 \quad if \quad \dot{q}_2 \neq 0 \qquad (12)$$

Hence q_1 and q_2 play the roles of position and ignorable coordinates, respectively, and therefore, the inertial motion of a particle on a smooth pseudosphere is unstable with respect to the ***ignorable*** coordinate, [1]. This instability known as orbital instability is not bounded by energy and it can persist indefinitely. As shown in [2], eventually orbital instability leads to stochasticity. Later on such motions were identified as chaotic.

b. Randomness in chaotic systems.

In this sub-section we present a sketch of general theory of chaos in context of origin of randomness starting with the flow generated by an autonomous ODE

$$\frac{dx_i}{dt} = V_i(\mathbf{x}), \quad i = 1,2,...m \qquad (13)$$

and compare two neighboring trajectories in *m*-dimensional phase space with initial conditions x_0 and $x_0 + \Delta x_0$ denoting $\Delta x_0 = w$. These evolve with time yielding the tangent vector $\Delta x(x_0, t)$ with its Euclidian norm

$$d(x_0, t) = \left\|\Delta x(x_0, t)\right\| \qquad (14)$$

Now the Liapunov exponent can be introduced as the mean exponential rate of divergence of two initially close trajectories

$$\tilde{\lambda}(x_0, w) = \lim_{\substack{t\to\infty \\ d(0)\to 0}} (\frac{1}{t}) \ln \frac{d(x_0, t)}{d(x_0, 0)} \tag{15}$$

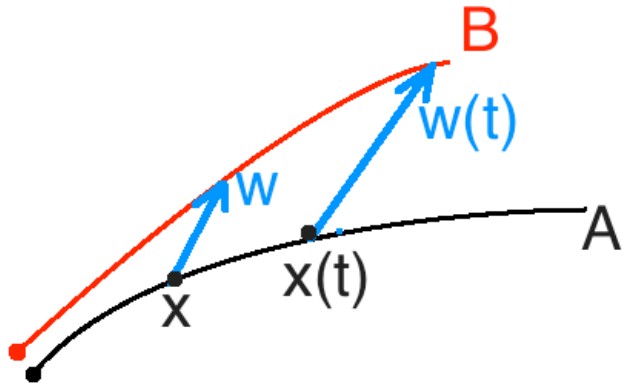
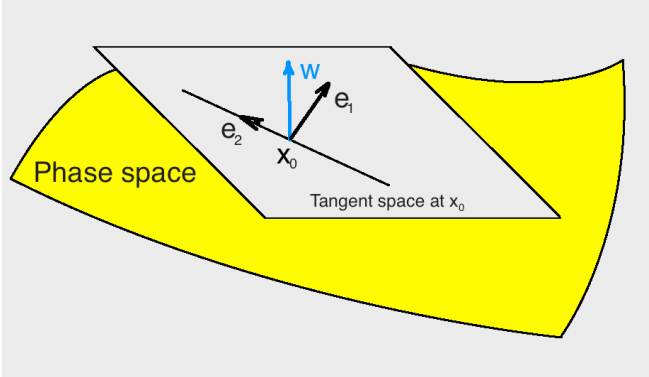


Figure 2. Two nearby trajectories that separate as time evolves.



Ficure 3. Tangent space for the Liapunov exponents.

Therefore in general the Lyapunov exponent cannot be analytically expressed via the parameters of the underlying dynamical system (as it can be done in case of inertial motion on a pseudosphere), and that makes prediction of chaos a hard task. However some properties of the Liapunov exponents can be expressed in an analytical form. Firstly, it can be shown that in an *m*-dimensional space, there exist *m* Liapunov exponents

$$\tilde{\lambda}_1 \geq \tilde{\lambda}_2 \ldots \geq \tilde{\lambda}_m \tag{16}$$

while at least one of them must vanish. Indeed, as follows from Eqs. (13) and (14), **w** grows only linearly in the direction of the flow, and the corresponding Liapunov exponent is zero. Secondly it has been proven that the sum of the Liapunov exponents is equal to the average phase space volume contraction

$$\sum_{i=1}^{m} \tilde{\lambda}_i = \Lambda_0 \tag{17}$$

where the instantaneous phase space volume contraction

$$\Lambda = \nabla \cdot \mathbf{V} \tag{18}$$

But

$$\Lambda_0 = \Lambda \tag{19}$$

when

$$\nabla \cdot \mathbf{V} = const \tag{20}$$

Therefore in case (20), the sum of the Liapunov exponents is expressed analytically

$$\sum_{i=1}^{m} \tilde{\lambda}_i = \nabla \cdot \mathbf{V} \tag{21}$$

Thus the result we extracted from the theory of chaos, which can be used for comparison to quantum randomness is the following: the origin of randomness in Newtonian mechanics is instability of ignorable variables that leads to exponential divergence of initially adjacent trajectories; this divergence is measured by Liapunov exponents, which form a discrete spectrum of numbers that must include positive ones.

For a system of N particles with coordinates X and velocities V, the following pair of first order differential equations may be written in Newton's notation as

$$F(X) = -\nabla U(X) = M\dot{V}(t)$$
$$V(t) = \dot{X}(t).$$

The potential energy function $U(X)$ of the system is a function of the particle coordinates X. It is referred to simply as the "potential" in physics, or the "force field" in chemistry. The first equation comes from Newton's laws; the force F acting on each particle in the system can be calculated as the negative gradient of $U(X)$.

5. Suppression of trajectories' divergence using negative diffusion.

a. Introduction. The approach proposed in this Section is based upon the removal of positive Liapunov exponents by introducing special control forces represented by negative diffusion, [23]. The role of these forces is to suppress the divergence of the trajectories corresponding to initial conditions that are different from the preset ones, without affecting the ''target'' trajectory that starts with the preset initial conditions. Since the control forces include probability densities of the state variables as new unknowns, the corresponding Liouville equation should be invoked for the closure. This equation is different from its classical version by additional nonlinear terms represented by negative diffusion, (see Figs. 27 and 28).

Consider a system of *n* first order ordinary differential equations with *n* unknowns

$$\dot{x}_i = f_i[\{x(t)\}, t], \quad \{x\} = x_1, x_2, \ldots x_n, \quad i = 1, 2, \ldots n$$

(4.37)

subject to initial conditions

$$x_i(0) = x_i^0$$

(4.38)

Due to finite precision, the values (4.38)) are not known exactly, and we assume that the error possesses some joint distribution

$$Err(X_i^0) = \rho(X_1^0,...X_n^0) = P_0$$

(4.39)

It is reasonable to assume that the initial conditions (4.38) coincide with the initial expectations i.e. that P has a maximum at $X_i^0 = x_i^0$, $i = 1,2,...n$. This means that

$$\frac{\partial P_0}{\partial X_0} = 0, \qquad \frac{\partial^2 P_0}{\partial X_i \partial X_j} < 0, \ i = 1,2,...n.$$

(4.40)

This is true for any symmetric initial density (for instance, the normal distribution) when the expected values have the highest probability to occur. The Liouville equation describing the evolution of the joint density P is

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho f) = 0, \quad F_i = F_i(\{x\},t) \quad P = P(\{X\},t)$$

(4.41)

Its formal solution

$$P = P_0 \exp(-\int_0^t \nabla \bullet f \, dV)$$

(4.42)

suggests that the flattening of the error distribution is caused by the divergence of the trajectories of the governing equations (4.37) from the target trajectory that starts with the preset initial conditions (4.38), Fig.27.

Remark. Here and below we make distinction between the random *variable x(t)* and its *values X* in probability space.

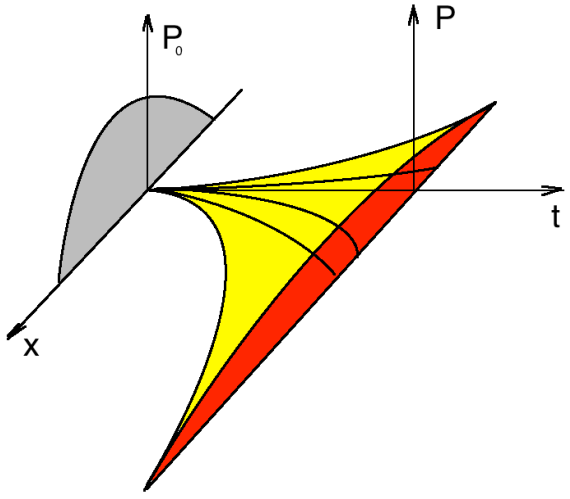


Figure 27. Uncontrolled evolutions of trsjectories.

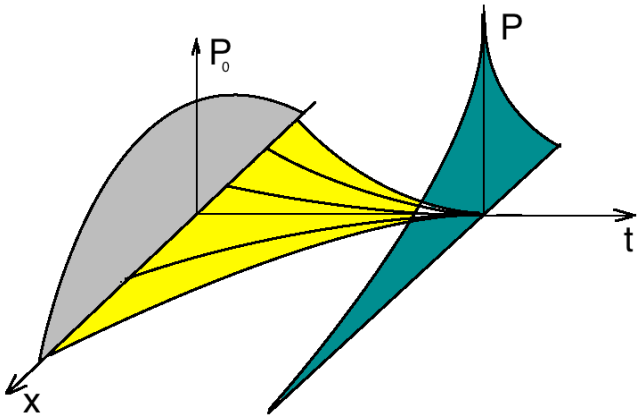


Figure 28. Controlled evolutions of trajectories.

b. Problem formulation. Let us apply the following control force to the system (4.37)

$$f_i = \alpha_i \frac{\partial}{\partial x_i} \ln P, \qquad \alpha_i > 0$$

(4.43)

Then the system (4.37) is modified to the following one

$$\dot{x}_i = f_i + \alpha_i \frac{\partial}{\partial x_i} \ln P, \tag{4.44}$$

that should be complemented by the corresponding Liouville equation

$$\frac{\partial P}{\partial t} + \sum_i \alpha_i \frac{\partial}{\partial X_i}\left(PF_i + \frac{\partial P}{\partial X_i}\right) = 0 \tag{4.45}$$

The coupled ODE-PDE equations of this type have been discussed in [23]. Here we will summarize only mathematical aspects of these systems.

Firstly, the force f_i makes the Liouville equation nonlinear, while ODE becomes dependent upon PDE. Secondly, this force introduces to PDE a negative diffusion that changes the type of the PDE from the hyperbolic to the parabolic one. At the same time, the behavior of the solution of Eq. (4.45) is fundamentally different from its Fokker-Planck analog.

Thirdly, as follows from Eq. (4.43), the force f_i ***does not affect*** the motion along that trajectory $x_i = x_i^*$ that has the maximum probability of occurrence since

$$\frac{\partial P}{\partial x_i}(x_i = x_i^*) = 0 \qquad (4.46)$$

and that property makes this force fictitious.

Before formulating the proposed model in the final form, we will consider a trivial, but instructive example.
The main purpose of this example is to demonstrate a suppression of trajectory divergence by a ***nonlinear negative*** diffusion rather than removal of positive Liapunov exponents.

c. Example. Let us consider an unstable linear ODE

$$\dot{x} = \varepsilon x, \qquad \varepsilon << 1 \qquad (4.47)$$

In this particular case, the expected trajectory is known in advance:

$$\bar{x} = 0 \qquad (4.48)$$

However, any small error in initial conditions leads to a different trajectory that diverge exponentially from those in Eq.(4.47):

$$x = x_0 \exp \varepsilon t \qquad (4.49)$$

Similar result follows from the corresponding Liouville equation:

$$\frac{\partial P}{\partial t} = -\varepsilon \frac{\partial}{\partial X}(PX) \qquad (4.50)$$

$$X = X_0 \exp \varepsilon t \qquad (4.51)$$

Let us introduce now the control force as

$$f_c = \sqrt{D}\frac{\partial}{\partial x}\ln P, \qquad (4.52)$$

where D is the variance

$$D(t) = \int_{-\infty}^{\infty} X^2 P(X,t) dX \qquad (4.53)$$

and obtain the following modifies version of Eq. (4.47)

$$\dot{x} = \varepsilon x + \sqrt{D}\frac{\partial}{\partial x}\ln P \qquad (4.54)$$

Due to this Liouville feedback, Eq. (4.50) is modified to the following Fokker-Planck equation

$$\frac{\partial P}{\partial t} = -\varepsilon \frac{\partial}{\partial X}(PX) - \sqrt{D}\frac{\partial^2 P}{\partial X^2} \tag{4.55}$$

Multiplying Eq.(4.55) by X, then using partial integration, one obtains for expectations the same

Eq. (4.50) and its solution (4.51).

Similarly one obtains for variances

$$\dot{D} = -2\sqrt{D} - \varepsilon D \approx 2\sqrt{D} \tag{4.56}$$

For the initial condition

$$D = D_0 \quad at \qquad t = 0 \tag{4.57}$$

the solution of Eq.(20) is

$$D = (\sqrt{D_0} - t)^2 \quad for \qquad t < \sqrt{D_0}, and \qquad D \equiv 0 \quad for \qquad t \geq \sqrt{D_0} \tag{4.58}$$

It is easily verifiable that the Lipchitz condition at $D=0$ is violated since

$$\frac{\partial \dot{D}}{\partial D} = -\frac{1}{\sqrt{D}} \to \infty \; at \qquad D \to 0 \tag{4.59}$$

As will be shown later, this property of the solution is of critical importance for multi-dimensional case.

Now the solution of the nonlinear version of the Fokker-Planck equation (4.55) can be approximated by the first term in the Gram-Charlier series represented by the normal distribution with the variance D. For the case close to a sharp initial value at $X=0$

$$P = \frac{1}{D\sqrt{2\pi}}\exp(-\frac{X^2}{2D^2}), \tag{4.60}$$

Substituting Eq.(4.60) (with reference to the solution (4.58) into Eq. (4.54) one obtains

$$\dot{x} = x[1 - \frac{1}{\sqrt{D_0} - t}] \tag{4.61}$$

whence for $x = x_0$ at $t=0$ the solution is

$$x = \frac{x_0}{D_0} e^t (\sqrt{D_0} - t)^2 \qquad 0 \leq t \leq D_0, \quad x \equiv 0 \quad t > D_0. \tag{4.62}$$

For sufficiently small variance of initial error distribution $D_0 << 1$, an exponential growth of initial error x_0 is totally eliminated after $t > \sqrt{D_0}$, Fig.29.

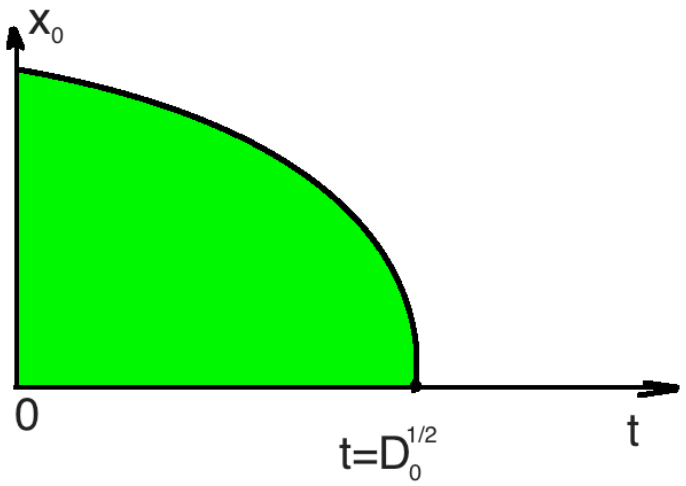


Figure 29. Suppression of instability.

It should be noticed that a finite time of approaching equilibrium is due to special properties of the terminal attractors discussed in Zak, M., 1970, 1993. One has to recall again that although the example we just considered is trivial, and Liapunov exponents does not play any role in it, the stabilization mechanism performed by the negative-diffusion-based Liouville-feedback forces is the same. It is also important to learn from this example that the true expected solution is given by Eq. (4.62) rather than by Eq. (4.51) despite the fact that Eq. (4.51) directly follows from the Liouville equation (4.55). Indeed, the solution (4.51) is identical to the original solution (4.49), and any initial error will grow exponentially. This means that both of these solutions are unstable *in the class of differentiable functions.*

But the same physical phenomenon described by Eq. (4.62) is stable in the *enlarged class of functions that includes stochastic components*. Obviously the stochastic components are found from the Stabilization Principle discussed in the previous section.

d. Comment on negative diffusion.

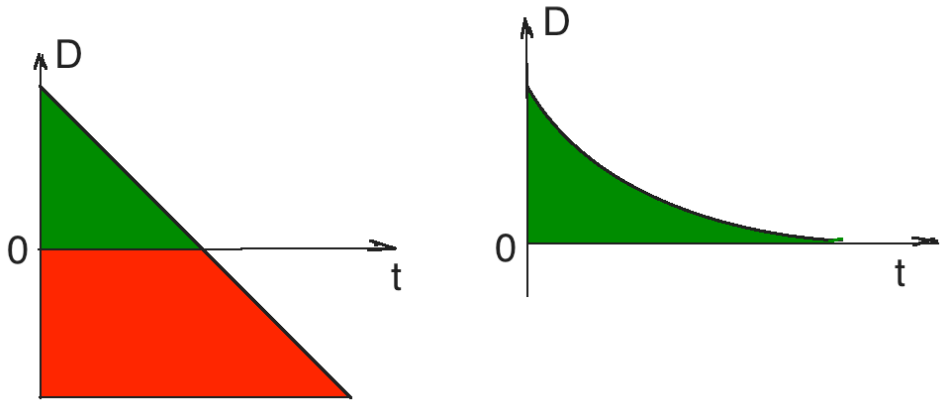
One may ask why the negative diffusion was chosen to be nonlinear. Let us turn to a linear version of the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = -\sigma^2 \frac{\partial^2 P}{\partial X^2}, \qquad \int_{-\infty}^{\infty} P\, dX = 1 \tag{4.63}$$

and discuss a negative diffusion in more details. As follows from the linear equivalent of Eq. (26)

$$\dot{D} = -2\sigma, i.e.\ D = D_0 - 2\sigma t < 0 \quad at \quad t > D_0/(2\sigma) \tag{4.64}$$

Thus, eventually the variance becomes negative, and that disqualifies Eq. (4.64) from being meaningful. As will be shown below, the initial value problem for this equation is ill-posed: its solution is not differentiable at any point. Therefore, a *negative diffusion must be nonlinear* in order to protect the variance from becoming negative, Fig.30.



Linear negative diffusion. **Nonlinear negative diffusion.**

Figure 30. Negative diffusion.

Since a parabolic PDE with negative diffusion coefficients is of fundamental importance for the proposed approach to the computation strategy, we will take a closer look at its properties associated with the so called Hadamard's instability, or the ill-posedness of the initial value problem. Without loss of generality, the analysis will be focused on the one-dimensional case.

Consider a parabolic PDE

$$\frac{\partial P}{\partial t} = -q^2 \frac{\partial^2 P}{\partial X^2} \tag{4.65}$$

subject to the following initial conditions

$$P^{00} = P\,|_{t=0} = \{\begin{matrix} \frac{1}{\lambda_0^2}\sin\lambda_0 X \quad if\ |X| \le X_0 \\ 0 \qquad\quad if \qquad |X| > X_0 \end{matrix}\} \tag{4.66}$$

with the parameter λ_0 being made as large as necessary,i.e

$$\lambda_0 \to \infty \tag{4.67}$$

The region of the initial disturbance can be made arbitrarily shrunk, i.e.

$$|X_0| \to 0 \tag{4.68}$$

The solution of Eq. (4.65) can be sought in the form

$$P = \frac{1}{\lambda_0^2} e^{\gamma \Delta t} \sin\lambda_0 X. \tag{4.69}$$

Substituting this solution into Eq. (4.65), one obtains

$$\lambda = q^2 \lambda_0^{\,2} \to \infty \quad at \qquad \lambda_0 \to \infty. \tag{4.70}$$

Thus, the solution of Eq. (4.65) subject to the initial conditions (4.66) is

$$P = \frac{1}{\lambda_0^2} e^{q^2 \lambda_0^2 \Delta t} \sin \lambda_0 X \tag{4.71}$$

This solution has very interesting properties: its modulus tends to infinity if

$$\lambda_0 \to \infty \tag{4.72}$$

within an arbitrarily short period of time Δt_0 and within an infinitesimal length around the point $X = X_0$. In other words, vanishingly small changes in the initial conditions lead to unboundedly large changes in the solution during infinitesimal period of time.

The result formulated above was obtained under specially selected initial conditions (4.66), but it can be generalized to include any initial conditions. Indeed, let the initial conditions be defined as

$$P|_{t=0} = P^*(X) \tag{4.73}$$

and the corresponding solution of Eq. (4.65) is

$$P = P^{**}(X,t) \tag{4.74}$$

Then, by altering the initial conditions to

$$P|_{t=0} = P^*(X) + P^{00}(X) \tag{4.75}$$

where $P^{00}(X)$ is defined by Eq. (4.66), one observes the preceding argument by superposition that vanishingly small change in the initial condition (4.73) leads to unboundedly large change in the solution (4.74) that occurs during an infinitesimal period of time. Such an unattractive property of the solution (that represents the Hadamard's instability) repelled scientists from using Eq. (4.65) as a model for physical phenomena. However, the situation becomes different if the variable P in Eq. (4.65) cannot be negative, i.e. when Eq. (4.65) is complemented by the constraint

$$P \geq 0 \tag{4.76}$$

This constraint is imposed, for instance, when ρ stands for the probability density, or for the absolute temperature. It is easily verifiable that the proof of the Hadamard's instability presented above fails if the constraint (41) is imposed, since negative values of ρ is essential for that proof. Thus, if the models of negative diffusion have attractors separating positive and negative areas of the solutions, they are free of the Hadamard's instability, and that what takes place in Eq. (25).

It should be emphasized that negative diffusion represents a major departure from both Newtonian mechanics and classical thermodynamics by providing a progressive evolution of complexity against the Second Law of thermodynamics.

e. General case. Based upon the example considered above, we can now specify the coefficients α_i in Eqs. (4.44), and (4.45)

$$\dot{x}_i = f_i + \sqrt{D_{ii}}\,\frac{\partial}{\partial x_i}\ln P, \tag{4.77}$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial X_i}(PF_i + \sum_i \sqrt{D_{ii}}\,\frac{\partial P}{\partial X_i}) = 0 \tag{4.78}$$

where D_{ii} are principal variances

$$D_{ii} = \int_{-\infty}^{\infty}\ldots\int_{-\infty}^{\infty}(X_i - \bar{X}_i)^2\,P(dX)^n \tag{4.79}$$

In order to verify the stabilizing effect of negative diffusion for *n*-dimensional case, let us linearize Eqs. (4.77) with respect to the initial state $x_i = 0$. Then the linearized versions of Eqs. (4.77) and (4.78) will be, respectively

$$\dot{x}_i = a_{ij}x_j + \sqrt{D_{ii}}\,\frac{\partial}{\partial x_i}\ln P, \quad a_{ij} = (\frac{\partial f_i}{\partial x_j})_{\substack{v \\ x_j=0}} \tag{4.80}$$

$$\frac{\partial P}{\partial t} + \frac{\partial}{\partial X}(\rho a_{ij}X_j + \sum_i \sqrt{D_{ii}}\,\frac{\partial \rho}{\partial X_i}) = 0 \tag{4.81}$$

An *n*-dimensional analog of Eq. (4.56) can be obtained by multiplying Eq.(4.81) by X_i and then using partial integration

$$\dot{D}_{ij} = -a_{il}D_{lj} - a_{jl}D_{li} - 2\sqrt{D_{ij}} \tag{4.82}$$

Let us first analyze the effect of terminal attractor and, turning to Eq.(4.82), start with the matrix $[\partial\dot{D}_{ij}/\partial D_{lk}]$. Its diagonal elements become infinitely negative when the variances vanish

$$\frac{\partial \dot{D}_{ij}}{\partial D_{ij}} = (-2a_{ij} - \frac{1}{\sqrt{D_{ij}}}) \to -\infty \qquad at \qquad D_{ii} \to 0 \tag{4.83}$$

while the off-diagonal elements are bounded. Therefore, due to the effect of terminal attractor (4.83), the system Eqs. (4.82) has infinitely negative characteristic roots, i.e. it is infinitely stable with respect to small errors regardless of the parameters a_{ij} of the original dynamical system (4.80). In addition to that, the terminal attractor (as well as any attractor) guarantees "impenetrability" of the state $D_{ii} = 0$, i.e. if the principle variances

initially were non-negative, they will never become negative, and that prevent ill-possedness of the problem for the PDE (4.78).

Thus, all the properties of the modified model discovered in one-dimensional case are preserved in the

n-dimensional case, namely: a simultaneous solution of the coupled ODE-PDE system (4.77) and (4.78) describes a stable "expected" motion regardless of the original instability.

f. Representation of higher moments. Although the expected (mean) values of the state variables play

an important role in description of postinstability motions, they do not expose the full dynamical picture.

Indeed, measured velocities of chaotic motions look truly random, and therefore, the behavior of the

higher moments is required within the framework of stochastic formalism. For that purpose, let us turn to

Eqs. (4.37) and introduce new variables

$$x_{ij} = x_i x_j \tag{4.84}$$

After trivial transformations, the system (4.37) can be rewritten in an equivalent form being expressed via new variables

$$\dot{x}_{ij} = f_{ij}(x_{11},...x_{nn}) \tag{4.85}$$

in which

$$f_{ij} = \sqrt{x_{jj}} f_i(\sqrt{x_{11}},...\sqrt{x_{nn}}\} + \sqrt{x_{ii}} f_j(x_{11},...\sqrt{x_{nn}}) \tag{4.86}$$

Let us now augment Eqs.(4.86) with the Liouville feedback similar to that in Eq.(4.77)

$$\dot{x}_{ij} = f_{ij} + \sqrt{D^*_{ijij}} \frac{\partial}{\partial x_{ij}} \ln P^*, \tag{4.87}$$

Then the corresponding Liouville equation will be similar to Eq. (4.78)

$$\frac{\partial P^*}{\partial t} + \frac{\partial}{\partial X_{ij}}(P f_{ij} + \sum_{ij} \sqrt{D^*_{ijij}} \frac{\partial P^*}{\partial X_i}) = 0 \tag{4.88}$$

where P^* and D^*_{ijij} are probability density and principal variances for the new variables. Solving Eqs.(4.87) and (4.78) simultaneously, one obtains the evolution of the expectations of the new state variables that are equivalent to the second moments of the old variables (see Eqs.(4.84))

$$\bar{x}_{ij} = \overline{x_i x_j} \tag{4.89}$$

It should be noticed that P and P^* are different: for instance, if initially P is normally distributed, P^* must be recalculated by applying the rules for the change of variables

(4.84); that is why the expectations and the second moments must be found from different equations.

The higher moments can be found in a similar way by introducing new variables x_{ijk}, x_{ijkl}, etc. Based upon the expectation and higher moments, one can reconstruct the joint probability distribution of state variables, and therefore, to obtain a complete information about dynamics of the underlying physical process in a *stable* form.

g. Computational complexity. Since the proposed approach, in general, can be implemented only by numerical simulations, its computational complexity becomes critical for a practical use. It should be emphasized that although our primary objective is to *stabilize the governing equations,* nevertheless our secondary objective is to make them practically tractable. As follows from the governing equations (27), and (28), one has to deal with $2n$ first order ODE and one second order parabolic PDE, and this PDE has exponential complexity in a sense that with a linear growth of the interacting bodies, the computational resources grow exponentially, and the problem becomes intractable. Indeed, Eq. (28) is a Fokker Planck equation for which the number of the independent variables is equal to the number of interacting bodies.

Here we will introduce a draft of the computational strategy for circumventing this obstacle by replacing simulation of Eq. (28) with direct collection statistics of the random trajectories. Assuming that the initial value of the joint probability density is a delta function, one can find all the state variables of the system (4.77), and (4.78) during a small time interval Δt. Repeating the same computations many times, one may obtain different results due to chaotic instability. These results can be used for collecting statistics and finding the joint probability density for the next small time interval, etc. It should be emphasized that the solution is obtained *without* exploiting the original PDE (28). The last property is very important since the complexity of the computing is coming from numerical solution of n-dimensional PDE. The price of this advantage is collection of statistics at each time step. Nevertheless, this procedure leads only to polynomial complexity, while computing or simulating an n-dimensional PDE has exponential complexity. Indeed, adopting Monte-Carlo approach applied for computation of multi-dimensional integrals, one can compute probability density by counting frequency of getting trajectories into preset areas, preset volumes, etc. while complexity of these simulations do not depend upon the problem dimensionality that is typical for Monte-Carlo methods, [24].

In particular, the computational complexity of integrating PDE is on the order of $(1/\varepsilon^2)^n$ that is, the reciprocal of the error threshold rose to a power equal to the number of variables that is exponential in n. In contradistinction to that, the resources for simulations by Monte-Carlo method is on the order of $(1/\varepsilon^2)$, i.e., they do not depend upon the dimensionality of the problem. Therefore, the complexity of the whole approach

is polynomial, and that is enormous advantage over standard approach to computing multi-dimensional Fokker-Planck equation. It should be noticed that the proposed approach is free of some limitations of the Monte-Carlo methods since success of the latter depends upon efficient implementations of multi-dimensional stochastic processes with prescribed density distribution, and that necessitates a fast and effective way to generate random numbers uniformly distributed on the interval [0,1]. It should be noticed that often-used computer-generated numbers are not really random, since computers are deterministic. In particular, if a random number seed is used more than once, one will get identical random numbers every time. Therefore, for multiple trials, different random number seeds must be applied. The proposed simulations approach does not need random number generator since *randomness is generated by the dynamical system itself via chaotic instability.* There is another advantage of proposed simulations: suppose that we are interested in behavior of the solution in a local region of the variables; then, in case of computing, one has to find the global solution first, and only after that the local solution can be extracted, while the last procedure requires some additional integrations in order to enforce the normalization constraints. On the other hand, in our case, one can project all the simulations onto a desired sub-space $j_\alpha \otimes j_\beta$ of the total space $j_1 \otimes ... j_l$ and directly obtain the local solution just disregarding the rest of the space. Similar approach has been applied to solution of the Madelung equation, [23].

6. Application to postinstability models.

a. General remarks.The proposed approach can be stated as follows: in order to find the solution
of a dynamical system (4.37) subject to the initial conditions (4.38) and avoid possible
computational errors due to exponential divergence of the neighboring trajectories, it is sufficient
to modify Eqs. (4.37) by applying a fictitious stabilizing force in the form of the Liouville feedback
(4.43) and to solve the system (4.77) subject to the same initial conditions (4.38), simultaneously
with the modified Liouville equation (4.78)
Obviously if stability of the system (4.37) in known in advance, the modification (4.77) and (4.78) is not necessary, although application of Eqs. (4.77) and (4.78) will only reaffirm this stability. However, in general, there is no analytical criterion that would predict chaos based only upon the system (4.37) without actual numerical runs. In view of that, the proposed approach seems quite universal.

b. Application to Lagrangian turbulence. In Section 2, the Lagrangian turbulence was described by
Eqs. (4.15)-(4.17) representing transition from Euler to Lagrange frames of reference. It was shown that
this is the simplest system of ODE that can has chaotic solutions. This phenomenon was identified with
the Lagrangian turbulence since the underlying Eulerian flow is laminar.

In order to apply the computational strategy developed in the previous Section, let us turn to Eqs. (4.15)-(4.17), and rewrite them in a dimensionless form. For that purpose, introduce the following variables

$$t = Tt^*,\ x = Xx^*,\ y = Yy^*,\ z = Zz^*$$
$$u = V_\infty u^*,\ v = V_\infty v^*,\ w = V_\infty w^*$$
(4.90)

Here T, L, and V_∞ are the scales of time, length and velocities.

Then Eqs. (4.15)-4.17) are written in a dimensionless form

$$S\frac{dx^*}{dt^*} = u^*(x^*, y^*, z^*)$$
(4.91)

$$S\frac{dy^*}{dt^*} = v^*(x^*, y^*, z^*)$$
(4.92)

$$S\frac{dz^*}{dt^*} = w^*(x^*, y^*, z^*)$$
(4.93)

where $S = \dfrac{L}{V\infty T}$ is the Strouhal number.

Now Eqs. (4.77) take the form

$$S\frac{dx^*}{dt^*} = u^*(x^*, y^*, z^*) + \sqrt{D_{xx}}\,\frac{\partial}{\partial x^*}\ln P$$
(4.94)

$$S\frac{dy^*}{dt^*} = v^*(x^*, y^*, z^*) + \sqrt{D_{yy}}\,\frac{\partial}{\partial y^*}\ln P$$
(4.95)

$$S\frac{dz^*}{dt^*} = w^*(x^*, y^*, z^*) + \sqrt{D_{zz}}\,\frac{\partial}{\partial z^*}\ln P$$
(4.96)

where

$$D_{xx} = \int_{-\infty}^{\infty}(X^* - \bar{X}^*)^2 P dX^* dY^* dZ^*$$
(4.97)

$$D_{yy} = \int_{-\infty}^{\infty} (Y^* - \bar{Y}^*_i)^2 P dX^* dY^* dZ^*$$

(4.98)

$$D_{zz} = \int_{-\infty}^{\infty} (Z^* - \bar{Z}^*_i)^2 P dX^* dY^* dZ^*$$

(4.99)

These equations should be complemented by the Liouville equation following from Eq. (4.78)

$$S\frac{\partial P}{\partial t^*} + \frac{\partial}{\partial X^*}(PU^* + \sqrt{D_{xx}}\frac{\partial P}{\partial X^*}) + \frac{\partial}{\partial Y^*}(PV^* + \sqrt{D''_{yy}}\frac{\partial P}{\partial Y^*}) + \frac{\partial}{\partial Z^*}(PW^* + \sqrt{D_{zz}}\frac{\partial P}{\partial Z^*}) = 0$$

(4.100)

The system of Eqs. (4.94)-4.96), and 4.100) is closed, and its solution, subject to the following initial conditions

$$x^* = x_0, \quad y^* = y_0, \quad z^* = z_0, \quad P = P_0 \quad at \quad t = 0$$

(4.101)

is to be sought in the form

$$\bar{x} = \bar{x}(x_0, y_0, z_0), \quad \bar{y} = \bar{y}(x_0, y_0, z_0), \quad \bar{z} = \bar{z}(x_0, y_0, z_0)$$

(4.102)

Here

x_0, y_0, z_0 are initial Cartesan coordinates of a trajectory of interest, and P_0 is the initial joint probability density of error in the values of these coordinates that can be chosen as a delta-function.

The solution (4.102) describes the equation of the sought trajectory averaged over time. The "real" trajectory may be not representable as a smooth curve due to chaotic instability. Recall that although the mean values of the coordinates $\bar{x}, \bar{y}, \bar{z}$ are not explicitly enter the system (4.91)-(4.93), they represent the limit values of x*,y*, and z*, respectively, as a result of the suppression of the trajectory divergence by the negative diffusion forces., Fig.31.

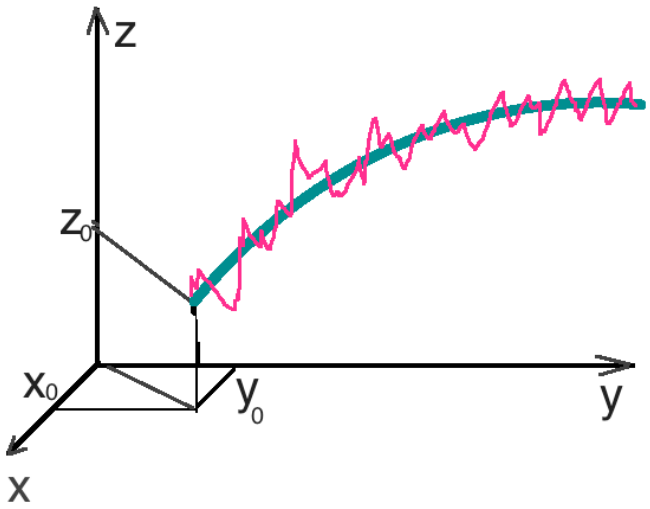


Figure 31. Chaotic and averaged trajectories**.**

Following Eqs. (4.84)-(4.88), one can formulate the problem for computing higher moments by introducing new variables and performing the same computational strategy.

c. Application to Navier-Stokes equations. Reformulation of the Euler and the Navier-Stokes equations
discussed in Chapter III did not cover a special case known as intermittency that is the irregular
alternation of phases of apparently periodic and chaotic dynamics. Intermittent behavior is commonly
observed in fluid flows that are near the transition to turbulence. In this sub-section we apply the approach
presented above to the intermittence turbulence described by the Navier-Stokes equation. In this case, prior to application of the proposed methodology, the Navier-Stocks equations must be approximated by a system of ODE. Such an approximation can be performed using finite differences, finite elements, or the Galerkin method. The relevance of the finite-dimensional approximation to solutions of the fluid dynamics has been successfully demonstrated by Lorenz, [25], who applied the Galerkin method to the Rayleigh- Benard convection model keeping only three Fourier components; as a result, he arrived at a strange attractor that now bears his name.
Let us illustrate the application of the Galerkin method to the Navier-Stokes equations. We will start with the following vector form

$$\rho(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\nabla\mathbf{v}) = -\nabla p + \nabla \bullet T + \mathbf{f}), \tag{4.103}$$

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{v}) = 0 \tag{4.104}$$

where $\mathbf{v}$ is the flow velocity, ρ is the fluid density, p is the pressure, T is the (deviatoric) stress tensor, and $\mathbf{f}$ represents body forces (per unit volume) acting on the fluid.

Let us represent Eqs. (4.103) and (4.104) in the following compressed form

$$\frac{\partial \mathbf{Q}(\mathbf{x},t)}{\partial t} = L(\mathbf{x})\mathbf{Q}(\mathbf{x},t) \tag{4.105}$$

where $\mathbf{Q}$ is m-dimensional vector that specifies the state of the fluid, $\vec{x}$ is the configuration space (with components x, y, and z,) and $L(\mathbf{x})$ is a time-independent, nonlinear differential operator. Applying Fourier decomposition into mode amplitudes to the vector $\mathbf{Q}$, one obtains

$$\mathbf{Q}(\mathbf{x},t) = \sum_k \mathbf{q}_k(t) e^{i\mathbf{k}\bullet\mathbf{x}} \tag{4.106}$$

where

$$\mathbf{q}_k(t) = \frac{1}{(2\pi)^3} \int d^3x \mathbf{Q}(\mathbf{x},t) e^{-i\mathbf{k}\bullet\mathbf{x}} \tag{4.107}$$

Inserting Eq. (4.106) into Eq.(4.105) and using the orthogonality of the exponential functions in (4.106), one obtains for each mode an equation of the form

$$\dot{\mathbf{q}}_k = \mathbf{F}_k(\mathbf{q}_1,...\mathbf{q}_k) \tag{4.108}$$

If only the first n modes are kept in the sum (4.106), then Eqs.(4.108) represent a set of mn first order ODE describing the evolution in time of the mode amplitude components.

Eqs. (4.108) are of the same form as Eqs (4.105), and their solution can be performed using the approach introduced above. The effectiveness of the Galerkin approach in *discretization* procedure of the Navier-Stokes equations follows from the fact that despite a sharp truncation of the Galerkin expansion, there are obvious *qualitative* similarities between the original PDE model and its tree-dimensional approximation representing the Lorenz attractor.

d. Application to n-body problem. Unlike the Navier-Stokes equations that describe dissipative motions,
the famous n-body problem describes conservative motions. But these two unsolved problems have a
fundamental property in common: driven by supersensitivity to initial condition, they develop chaotic
motions, and it turns out that the proposed methodology can be applied to both of them. The n-body

problem is a classic astronomical and physical problem that naturally follows from the two-body problem
first solved by Newton in his *Principia* in 1687. The efforts of many famous mathematicians have been
devoted to this difficult problem, including Euler and Lagrange (1772), Jacobi (1836), Hill (1878),
Poincaré (1899), Levi-Civita (1905), and Birkhoff (1915). However, despite centuries of exploration,
there is no clear structure of the solution of the general *n*- or even three-body problem as there are no
coordinate transformations that can simplify the problem, and there are more and more evidences that, in
general, the solutions of *n*-body problems are chaotic. Failure to find a general analytical structure of the
solution shifted the effort towards numerical methods. Many ODE solvers offer a variety of advance
numerical methods for the solution. However due to the sensitivity of the solution to initial errors,
different runs produce different results that is typical for chaotic phenomena. The governing equations of
n-body problem can be written in the form of *2n* ODE of the first order

$$\dot{\mathbf{v}}_i = -G\sum_{j=1,j\neq i}^{n} m_i \frac{\mathbf{r}_{ij}}{r_{ij}^3}, \qquad \dot{\mathbf{r}}_i = \mathbf{v}_i, \qquad \text{i=1,2,…n}$$

(4.109)

Here ***r,v*** and *m* are positions, velocities and masses of the bodies centers, and $\mathbf{r}_{ij}$ is the distance between these centers. The sensitivity of solutions of these ODE's leading to chaos is measured by the Lyapunov exponents. Quantitatively, two trajectories in phase space with initial separation $\delta Z_0(t)$ diverge as

$$|\delta Z| \approx e^{\lambda t} |\delta Z_0|$$

(4.110)

where λ is the Lyapunov exponent. A typical value of the positive Lyapunov exponent in a three body problem is $\lambda \approx 0.5$. Although the divergence that is associated with the Lyapunov instability is weaker that the Hadamard instability, it still leads to chaos. Here we will apply a new approach to solution of *n*-body problem proposed in this Chapter. First of all, the system (4.109) should be presented in the form equivalent to Eqs. (4.77), (4.78)

$$\dot{v}_i^k = -G\sum_{j=1,j\neq i}^{n} m_i \frac{r_{ij}^k}{r_{ij}^3} + \sqrt{D_{ii}^k}\,\frac{\partial}{\partial v_i^k}\ln P, \qquad i=1,2,...n; \quad k=1,2,3.$$

(4.111)

$$\dot{r}_i^k = v_i^k + \sqrt{\tilde{D}_{ii}^k}\,\frac{\partial}{\partial r_i^k}\ln P, \qquad i=1,2...n; \quad k=1,2,3.$$

(4.112)

$$\frac{\partial P}{\partial t} + \sum_{k=1}^{3}\sum_{i=1}^{n}\{\frac{\partial}{\partial V_i^k}[P(-G\sum_{j=1,j\neq i}^{n} m_i \frac{R_{ij}^k}{R_{ij}^3}) + \frac{\partial (PV_i^k)}{\partial R_i^k}] +$$

$$+\frac{\partial}{\partial V_i^k}(\sqrt{\tilde{D}_{ii}^k}\,\frac{\partial P}{\partial V_i^k}) + \frac{\partial}{\partial R_i^k}\sqrt{D_{ii}^k}\,\frac{\partial P}{\partial R_i^k})\} = 0$$

(4.113)

where r_i^k is the k^{th} Cartesian projection of the radius-vector of the i^{th} body

v_i^k is the k^{th} Cartesian projection of the velocity vector of the i^{th} body

r_{ij}^k is the k^{th} Cartesian projection of the radius-vector of the distance between the i^{th} and the j^{th} bodies, and

$$D_{ii}^k = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}(V_i^k - \bar{V}_i^k)^2 P dW \tag{4.114}$$

$$\tilde{D}_{ii}^k = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}(X_i^k - \bar{X}_i^k)^2 P dW \tag{4.115}$$

Here W is the volume of the probability space

$$dW = dX_1 dX_2 dX_3 dV_1 dV_2 dV_3 \tag{4.116}$$

The last terms in Eqs. (4.111) and (4.112), and the second line in Eq. (4.114) represent the effect of the fictitious forces in the form of the Liouville feedback.

7. Summary.

In this Chapter, the Lagrangian turbulence is defined as postinstability motion of individualized trajectories of a fluid generated by a laminar flow. The formulation of L-turbulence is reduced to a system of three nonlinear ODE describing kinematics of transition from Euler's to Lagrange's frames of reference. It has been demonstrated that the complexity of this ODE is equivalent to that of the simplest chaotic systems like a Lorentz attractor. Application of the Stabilizaion Principle to Lagrangian turbulence with generalization to the Navier-Stokes equations and n-body problems are discussed.

A general approach to representation of postinstability motions in dynamics is the central objective of this Chapter. The approach is based upon introduction of stabilizing forces that couple equations of motion and the evolution of the probability density of errors in

initial conditions. These stabilizing forces create a powerful terminal attractor in the probability space that corresponds to occurrence of the target trajectory with the probability one. In configuration space, this effect suppresses exponential divergence of the close neighboring trajectories without affecting the target trajectory. As a result, the postinstability motion is represented by a set of functions describing the evolution of the statistical invariants such as expectations and higher moments, while this representation is stable. General analytical proof has been introduced. Since the proposed approach is not restricted by any special assumptions about the original dynamical system, it can be applied to both conservative and dissipative systems. The main applications for conservative systems are in celestial mechanics as well as in molecular dynamics (for instance, many-body problems). The broad class of dissipative systems to which the proposed approach can be applied includes chaotic attractors and turbulence.

It should be noticed that the proposed approach combines several departures from the classical methods. Firstly, it introduces a nonlinear version of the Liouville equation that is coupled with the equation of motion (in Newtonian dynamics they are uncoupled). Secondly, it introduces terminal attractors characterized by violation of the Lipschitz conditions (in Newtonian dynamics as well as in theory of differential equations these conditions are preserved). Finally, the idea of a forced stabilization of unstable equations follows from the Stabilization Principle formulated in Chapter II. This is the most fundamental conceptual departure from the classical approach to mathematical modeling.

Referenses.

1. Alder, B. J.; T. E. Wainwright (1959). "Studies in Molecular Dynamics. I. General Method". *J. Chem. Phys.* **31** (2): 459.Bibcode:1959JChPh..31..459A.doi:10.1063/1.1730376.

2. Jump up to: Rahman, A. (19 October 1964). "Correlations in the Motion of Atoms in Liquid Argon". *Physical Review* **136** (2A): A405–A411.Bibcode:1964PhRv..136..405R.doi:10.1103/PhysRev.136.A405.

3. Skeel, R. SIAM J Sci Comput. 2009 Jan 16; 31(2): 1363–1378.
4. J. Synge, 1926, On the geometry of dynamics, Phil. Trans. R. Sos. Lond., Ser.A 226, 31-106.
5. V. Arnold, 1988, Mathematical methods of classical mechanics, Springer, New York