Short communication

Model of the diffusion process in a nanostructured system as a generator of pseudorandom sequences

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DOI: 10.26456/pcascnn/2026.18.296

Abstract: Complex random number generators that combine rapid pseudorandom sequence generation with hardware entropy sources have numerous practical applications in stochastic process modeling, machine learning, and information security. This paper presents a method for generating pseudorandom sequences based on a physical model of particle diffusion within a nanoscale periodic structure featuring a nonlinear potential and thermal noise, which serve as sources of dynamic chaos. The sequence of thermally activated transitions between potential minima exhibits irregular and chaotic behavior. The sequence generation is achieved through the digitalization of the particle's stochastic motion along the energy landscape of the nanostructure. Particle diffusion in a nanostructured medium is described by the Langevin equation and is integrating by using the Verlet method. Additionally, a software implementation of the suggested algorithm is provided in the Ruby programming language. The obtained results demonstrate the potential for using a «pseudophysical» approach, which is based on nonlinear potentials of various physical natures, as a viable alternative to a «purely mathematical» methodology in the tasks involving the generation of random number sets.

Keywords: nanostructures, diffusion, nonlinear potential, dynamic chaos, pseudorandom numbers.

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УДК 544.723, 538.9, 004.056.55, 004.421

Краткое сообщение

Модель диффузии в наноструктурированной системе как генератор псевдослучайных последовательностей

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DOI: 10.26456/pcascnn/2026.18.296

Аннотация: Комбинированные генераторы случайных чисел, сочетающие быструю генерацию псевдослучайных последовательностей и аппаратные источники энтропии, имеют массу практических приложений в сфере моделирования стохастических процессов, машинном обучении и информационной безопасности. В работе продемонстрирован метод генерации псевдослучайных последовательностей на основе физической модели процесса диффузии частицы в наноразмерной периодической структуре с нелинейным потенциалом и тепловым шумом, выступающими источником динамического хаоса. Последовательность термически активированных переходов между минимумами потенциала носит нерегулярный и хаотический характер, генерация результирующей последовательности осуществляется на основе оцифровывания стохастического блуждания частицы по энергетическому ландшафту наноструктуры. Диффузия частицы в наноструктурированной среде описывается уравнением Ланжевена, интегрируемого методом Верле. Приведена программная реализация предложенного алгоритма на языке программирования Ruby. Полученные результаты

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демонстрируют потенциал использования «псевдофизического» подхода, основанного на нелинейных потенциалах различной физической природы, в качестве работоспособной альтернативы «чисто математической» методологии в задачах генерации наборов случайных чисел.
Ключевые слова: наноструктуры, диффузия, нелинейный потенциал, динамический хаос, псевдослучайные числа.

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Поступила в редакцию/received: 01.01.2026; после рецензирования/revised: 30.01.2026; принята/accepted: 05.02.2026.

1. Introduction

Random number generators are devices or algorithms capable of producing sequences of numbers whose order is inherently unpredictable. Their primary purpose is to provide sources of unpredictability for various applications, ranging from scientific simulations to information security [1]. Without them, modern cryptography, reliable software testing, and certain types of computer games would be impossible.

A key distinction exists between truly random and pseudorandom number generators. The fundamental difference lies in their sources of unpredictability. Pseudorandom number generators are entirely deterministic systems [2]. They are most often implemented in software, generating sequences of numbers that appear statistically indistinguishable from truly random sequences to an «external observer». However, such sequences are uniquely determined by an initial value known as a «seed». True randomness, on the other hand, is achieved exclusively through hardware generation based on processes that are inherently non-deterministic and fundamentally unpredictable [3]. Sources of entropy for such hardware generators may include quantum phenomena – such as spontaneous photon emission [4] – classical noise [5], thermal noise [6] in resistors or *p-n* junctions, or, with certain limitations, «anthropic» processes [7, 8], such as the precise timing of keystrokes or the pattern of mouse movements.

In practice, a hybrid approach is often employed, combining the advantages of both methods. In this scheme, a high-speed pseudorandom number generator produces the main data stream, while its operation is periodically interrupted, and the initial state is updated with new «portions» of entropy obtained from a physical generator. This allows for the high generation speed required by various applications to be achieved, while simultaneously maintaining an adequate level of cryptographic strength. Furthermore, the development of such an approach assumes cost reduction and hardware optimization for entropy generators, the implementation of methods for cryptographic hashing of the output sequences, and the utilization of less «obvious» sources of pseudorandom sequences (as alternatives to traditional

linear congruential methods [9] or, for example, Mersenne Twisters [10]). The role of such generators can be played by models of physical processes exhibiting chaotic dynamics [11], where selecting initial conditions from a certain range yields a randomly scattered set of trajectory characteristics in phase space, observable externally. Examples of these processes include a double-suspension pendulum, the gravitational interaction among three bodies, or the motion of a test particle in a Kerr gravitational field. In the present study, such a process is modeled by diffusion in a nanoscale structure, described by the Langevin equation [12, 13] with a nonlinear periodic potential that characterizes a nanoscale lattice, with stochasticity introduced by thermal noise [14]. The potential forms a periodic sequence of energy minima and barriers. Each minimum corresponds to a stable state, while the barriers define the activation energy required for the particle to transition to the adjacent potential well. The particle is influenced by two competing factors: the deterministic component tends to localize it at the nearest energy minimum, whereas stochastic thermal fluctuations induce instability in its position. When the energy of this thermal vibrations reaches a sufficient level to surmount the potential barrier, an activated transition to the neighboring well occurs. The nonlinearity of the potential gives rise to the irregular, chaotic nature of these transitions, which exhibit exponential sensitivity of the particle's trajectory to initial conditions. Any small variation in initial coordinates or momentum results in a qualitative change in the temporal characteristics of the transition sequence between potential wells. This chaotic sequence of transitions is employed to generate random numbers by «digitizing» the stochastic wandering of the particle over the nanostructure's energy landscape. The approach presented below illustrates the potential for use as a pseudorandom sequence generator, a capability shared by numerous nonlinear dynamic processes of fundamentally different physical origins [15, 16].

2. The mathematical basis of the entropy generator

The motion of a particle in a nanostructured medium is described by the Langevin equation as follows:

$$m\left(d^2\mathbf{r}/dt^2\right) = -\gamma\left(d\mathbf{r}/dt\right) - \nabla U\left(\mathbf{r}\right) + \sqrt{2\gamma k_B T}\cdot\xi\left(t\right),$$

where $m\left(d^2\mathbf{r}/dt^2\right)$ represents an inertial term; $-\gamma\left(d\mathbf{r}/dt\right)$ models the resistance of the environment; $-\nabla U\left(\mathbf{r}\right)$ is the force resulting from the interaction with walls; $\sqrt{2\gamma k_B T}\cdot\xi\left(t\right)$ is the force caused by thermal fluctuations.

For the problem described above, it suffices to consider the one-dimensional case x. An extended periodic potential is employed in the following form:

$$U\left(x\right) = U_0\left[\cos\left(2\pi x/d\right) + \varepsilon\cos\left(4\pi x/d\right)\right],$$

where the first term describes the fundamental periodicity of the atomic lattice, and the second term accounts for anharmonic corrections. d is the spatial period. The force acting on the particle is calculated as the negative gradient of the potential:

$$F(x) = -dU(x)/dx = (2\pi U_0/d)\left[\sin(2\pi x/d)4 + 2\varepsilon\sin(4\pi x/d)\right].$$

Numerical integration is performed using the Verlet method [17], which is commonly employed for stochastic systems:

$$x_{n+1} = x_n + v_n\Delta t + a_n\Delta t^2/2, \quad v_{n+1} = v_n + (a_n + a_{n+1})\Delta t/2,$$

where x_n, v_n, a_n are the coordinate, velocity and acceleration of the particle at step n while $a_n = (-\gamma v_n + F(x_n) + noise)/m$, Δt is the time step.

The software implementation of the model is performed using «natural» units: the length unit is set to d=1,0 nm; the energy unit is $E = k_B T_{room}$=4,1·10^{-21} J (corresponds to room temperature); the mass unit is $m \sim 3\cdot10^{-26}$ kg (mass of water molecule); the time step is $\tau = \sqrt{md^2/U_0}$ (characteristic time of particle oscillations in a potential well). For stream generation of pseudo-random sequences, the values of the calculation parameters (γ, ε, «temperature» $k_B T$ (as well as the time step Δt) expressed in «natural» units) can be varied within a certain range to achieve greater variability in the resulting sets. The following values are used in the example below: $k_B T$ = 0,3 in units of E (the temperature value balances deterministic and chaotic dynamics: it is high enough to overcome small barriers, but not so high that noise dominates); $U_0 = 5k_B T$ = 1,5 (in units of E, the barrier is sufficiently high to trap particles but not so high as to prevent thermally activated transitions); ε = 0,25 (the value is sufficient to break the symmetry of the potential, resulting in additional minima and maxima, while the phase space corresponding to this value contains both chaotic and regular trajectories); Δt = 0,001(in units of τ, the time step is sufficiently small to resolve fast oscillations). γ = 0,05 (in units of m/τ). An estimate of the Lyapunov exponent for these values yields a value on the order of 0,1 (in units of τ^{-1}) which corresponds to the value of 3,65·10^{10} s^{-1} and indicates the chaotic behavior (the exact value requires a numerical solution of the variational equations combined with the Langevin equation).

Pseudo-random numbers are generated by converting the chaotic trajectory of a particle into a bit sequence. After several steps of integrating the Langevin equation – describing the motion of a particle within the nonlinear potential of a nanostructure – the current position of the particle is obtained. This position is normalized to the range of [0, 1], and its fractional part is successively multiplied by 2. Each multiplication yields one bit: if the result exceeds 1, a bit of 1 is extracted; if less than 1, a bit of 0. Repeating this process 32 times produces a 32-bit random number. The force $\xi(t)$ associated with

thermal fluctuations in the suggested algorithm is generated using the Box-Muller transform [18], which is convenient for software implementation within the chosen framework (this is not the only possible approach; alternatives include the Marsaglia-Bray modification, the Ziggurat algorithm for efficient Gaussian sampling, or built-in generators of classical Gaussian white noise available in various software environments, which produce signals with zero mean and delta correlation.) The factor $\sqrt{2\gamma k_B T}$ is introduced to ensure that the fluctuation-dissipation theorem is satisfied.

The described approach is implemented programmatically using the Ruby programming language [19], which offers an optimal balance between code brevity and readability, along with a minimal amount of *boilerplate* code among object-oriented languages suitable for such applications.

The implementation of the suggested algorithm in the Ruby language is provided in the following code block:

```
class NanoRNG
  def initialize(m=1.0,γ=0.05,u=1.5,a=1.0,ε=0.25,k=0.3,dt=0.001)
    @m,@γ,@u,@a,@ε,@k,@dt,@x,@v,@rng=m,γ,u,a,ε,k,dt,rand*a,0.1*rand,Random.new
    @cache=nil
  end
  def n; @cache||(u1,u2=@rng.rand,@rng.rand; u1=1e-10 if u1==0; r=Math.sqrt(-2*Math.log(u1));
t=2*Math::PI*u2; @cache=r*Math.sin(t); r*Math.cos(t))end
  def f(x) (2*Math::PI*@u/@a)*(Math.sin(2*Math::PI*x/@a)+2*@ε*Math.sin(4*Math::PI*x/@a))end
  def s
    rf=Math.sqrt(2*@γ*@k/@dt)*n
    df=f(@x)
    a_now=(-@γ*@v+df+rf)/@m
    x_new=@x+@v*@dt+0.5*a_now*@dt*@dt
    v_half=@v+0.5*a_now*@dt
    nf=f(x_new)
    a_new=(-@γ*v_half+nf+rf)/@m
    @v=v_half+0.5*a_new*@dt
    @x=x_new
    @x-=@a if@x>=@a
    @x+=@a if@x<0
  end
  def r;10.times{s};t=@x/@a;b=0;32.times{t*=2;b=(b<<1)|t.to_i;t-=t.to_i};b end
end
g=NanoRNG.new
p 10.times.map{g.r}
```

In Monte Carlo simulations, testing, or game environment generation – where the statistical properties of the resulting sequences are sufficient – the suggested algorithm can be used directly. However, if cryptographic security is required, the output sequence can be processed with cryptographic hashing (for example, using an algorithm from the SHA family) and combined with entropy generated using hardware sources.

3. Conclusion

The mechanism of transition to chaos in a system with given parameters is determined by the joint action of several factors [20, 21]. The potential nonlinearity, characterized by the parameter $\varepsilon = 0{,}25$, disrupts the harmonic oscillations of the particle within the potential well. This results in a complex structure of overlapping resonances in the phase space of the system. When the trajectory of a particle enters the interaction zone between these resonances, its motion becomes highly unstable. Dissipation, characterized by the parameter $\gamma = 0{,}05$ (expressed in «natural» units), plays a crucial role in the formation of a strange attractor by compressing the phase volume, which is essential for establishing a stationary chaotic regime. In this case, thermal fluctuations with the energy of $k_B T = 0{,}3$ (in units of E), which is approximately one fifth of the potential barrier height, constantly drive the system out of equilibrium. These fluctuations serve as a «stochastic bridge», triggering transitions of the particle between different regions of phase space and enabling its movement between regular and chaotic zones.

The critical condition is expressed as the ratio of the potential barrier height to the thermal energy, given by $U_0 / k_B T \approx 5$. At this ratio, the system approaches a threshold where thermally activated transitions between wells become relatively frequent but do not yet dominate the deterministic dynamics. This creates conditions for intermittency – a regime in which laminar phases of regular motion within potential wells alternate with turbulent bursts of chaotic transitions between wells. In this regime, the phase portrait exhibits a complex fractal structure [21-24]. Sensitivity to initial conditions manifests itself through the exponential divergence of trajectories originating from points arbitrarily close in phase space, a hallmark characteristic of deterministic chaos [14].

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