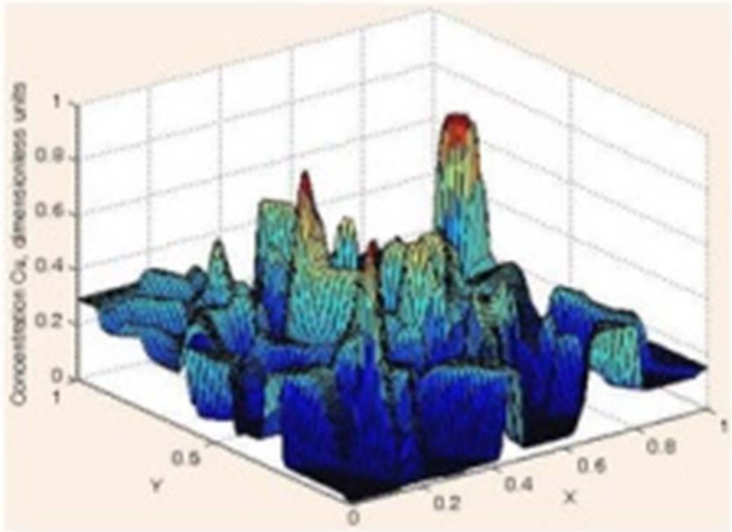


Комп'ютерне моделювання задач прикладної математики

Дифузія невзаємодіючих частинок. Рівняння Ланжевена

Лабораторна робота 1

Рівняння Ланжевена

$i = 1 \ldots N$

$$\frac{dx_i}{dt} = f(x_i) \qquad \frac{dx_i}{dt} = \frac{x_n - x_{n-1}}{\Delta t} \qquad x_n = x_{n-1} + f(x_{n-1})\Delta t$$

$$\frac{dx_i}{dt} = \xi(t) \qquad x_n = x_{n-1} + \sqrt{D\Delta t}\xi(t)$$

$$\xi = \sqrt{-2\ln(\zeta_1)}\sin(2\pi\zeta_2)$$

```
double ksi()
{
double p1=rand()/(RAND_MAX+1.0);
double p2=rand()/(RAND_MAX+1.0);
if (!p1) p1=1e-10;
return sqrt(-2*log(p1))*sin(2.0*pi*p2);
}
```

Рівняння Ланжевена

```
While(t < t_fin)
{

For(i=0..N)

X[i]+=sqrt(D*dt)*ksi()

If(t > t_write)
{
  x_mean = 0;
 for(i=0..N)
{
    x_mean+=x[i]
   x2_mean+=x[i]*x[i];
}
x_mean=x_mean/N;
x2_mean=x2_mean/N;
Delta = x2_mean-x_mean*x_mean;
Fprntf(   t, Delta)
t_write+=dt_write
}
```

$$i = 1 \ldots N$$

$$\frac{dx_i}{dt} = \frac{x_n - x_{n-1}}{\Delta t}$$

$$x_n = x_{n-1} + f(x_{n-1})\Delta t$$

$$\frac{dx_i}{dt} = f(x_i)$$

$$\boxed{\begin{gathered} \frac{dx_i}{dt} = \xi(t) \\ x_n = x_{n-1} + \sqrt{D\Delta t}\,\xi(t) \\ \xi = \sqrt{-2\ln(\zeta_1)}\sin(2\pi\zeta_2) \end{gathered}}$$

$$\langle(\delta x)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$$

Рівняння Ланжевена

$$\frac{dx_i}{dt} = f(x_i) + \xi(t)$$

$$x_n = x_{n-1} + f(x_{n-1})\Delta t + \sqrt{D\Delta t}\xi(t)$$

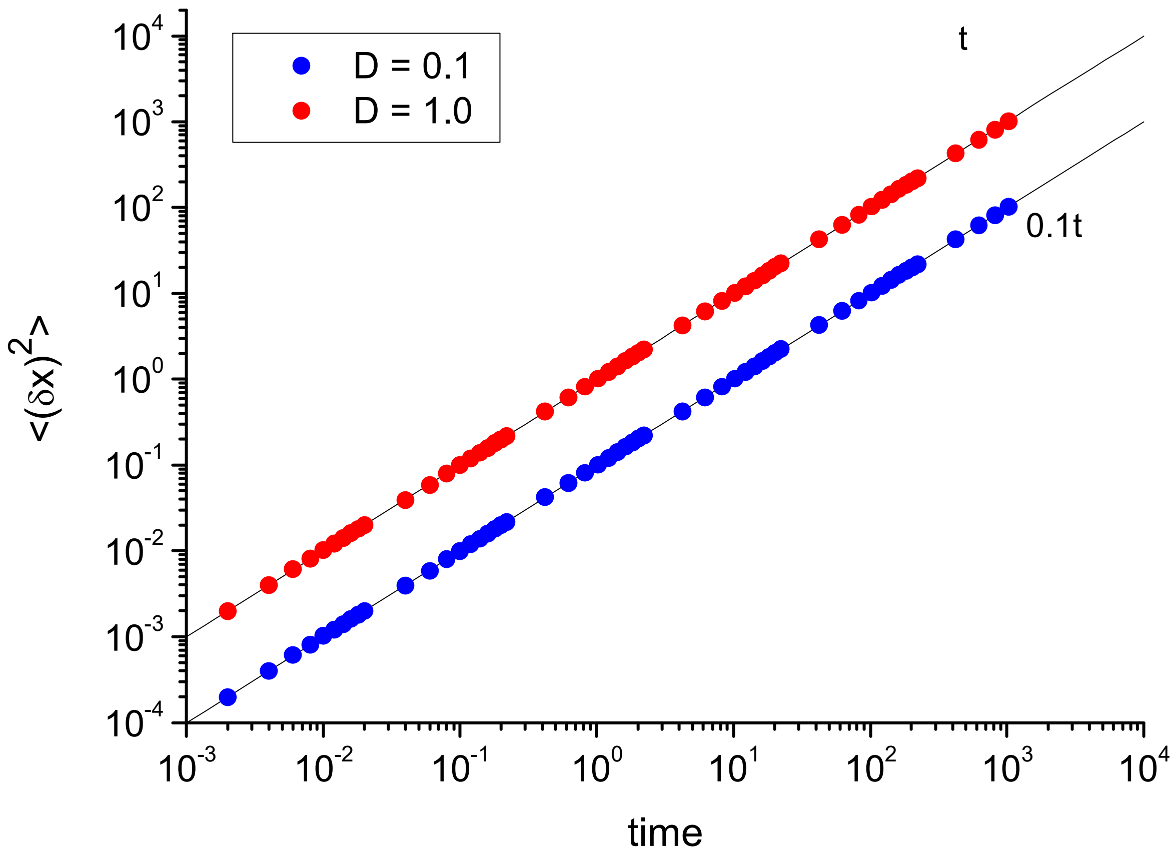
$$\xi = \sqrt{-2\ln(\zeta_1)}\sin(2\pi\zeta_2)$$

```
double ksi()
{
double p1=rand()/(RAND_MAX+1.0);
double p2=rand()/(RAND_MAX+1.0);  if (!p1)
p1=1e-10;
return sqrt(-2*log(p1))*sin(2.0*pi*p2);
}
```

Рівняння Ланжевена

Task 1

$$\mathrm{f(x)} = 0 \qquad x_n = x_{n-1} + \sqrt{D\Delta t}\,\xi(t)$$

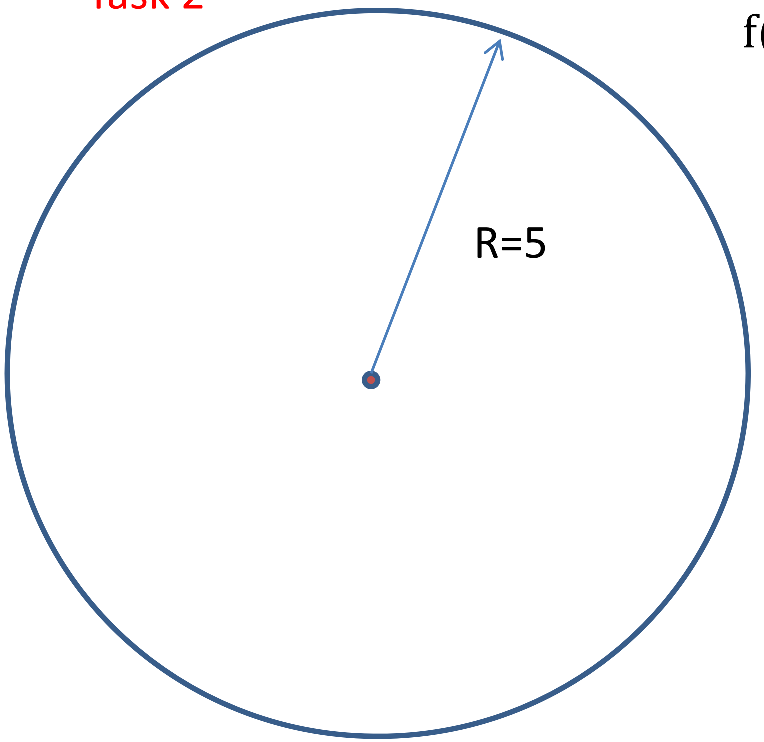


$N=10^4$

$\Delta t = 0.002$

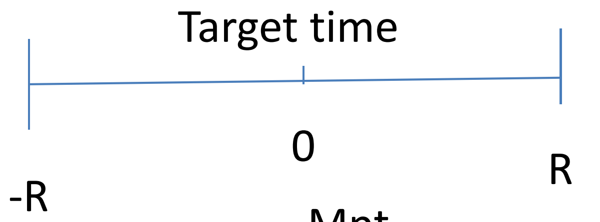
Рівняння Ланжевена

Task 2



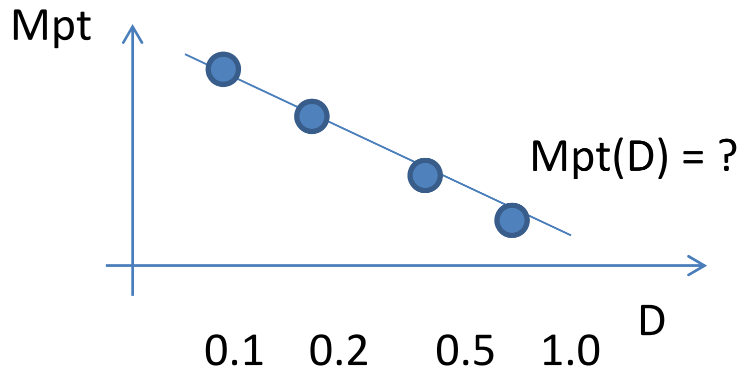
$$f(x) = 0$$

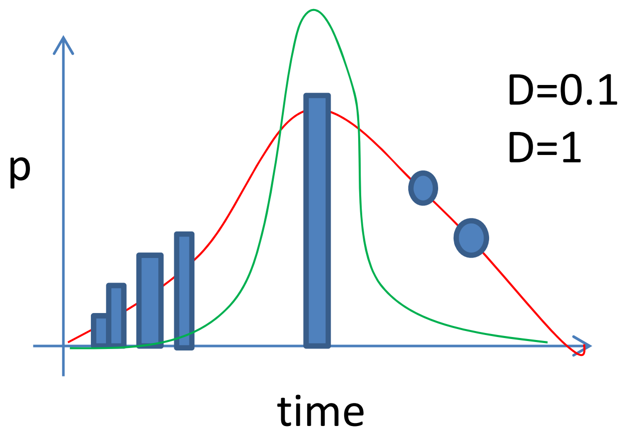
$$x_n = x_{n-1} + \sqrt{D\Delta t}\,\xi(t)$$

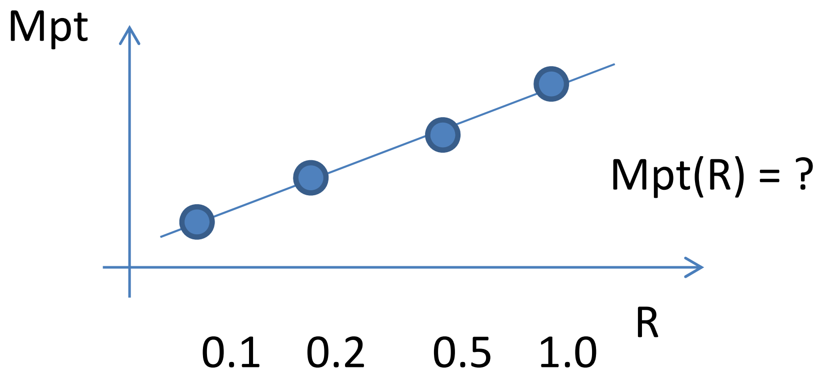


$N=10^4$

$\Delta t = 0.002$







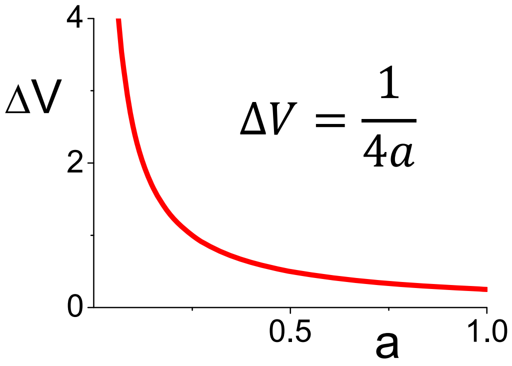
Task 3

Рівняння Ланжевена

$$x_n = x_{n-1} + f(x_{n-1})\Delta t + \sqrt{D\Delta t}\,\xi(t)$$

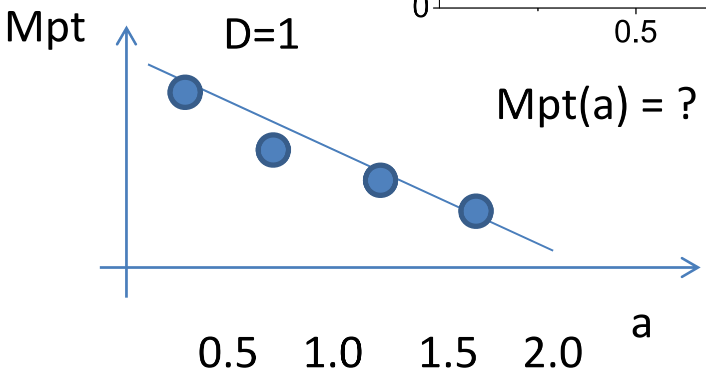
$$f(x) = -\frac{dV}{dx}$$

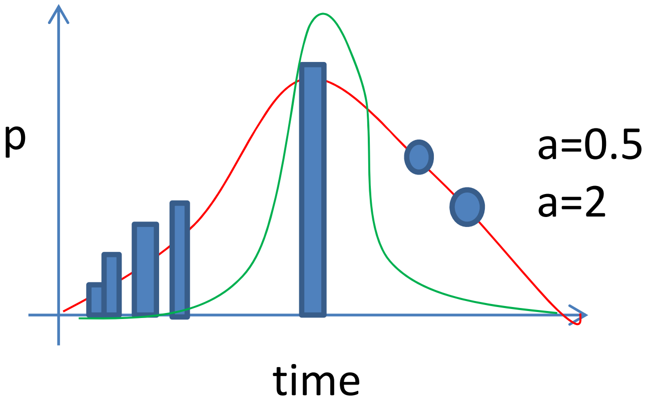
$$V = ax^4 - x^2$$

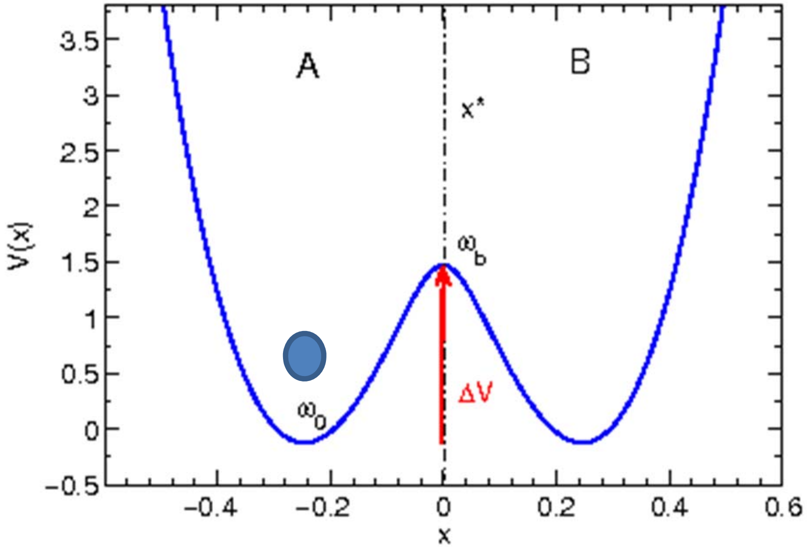


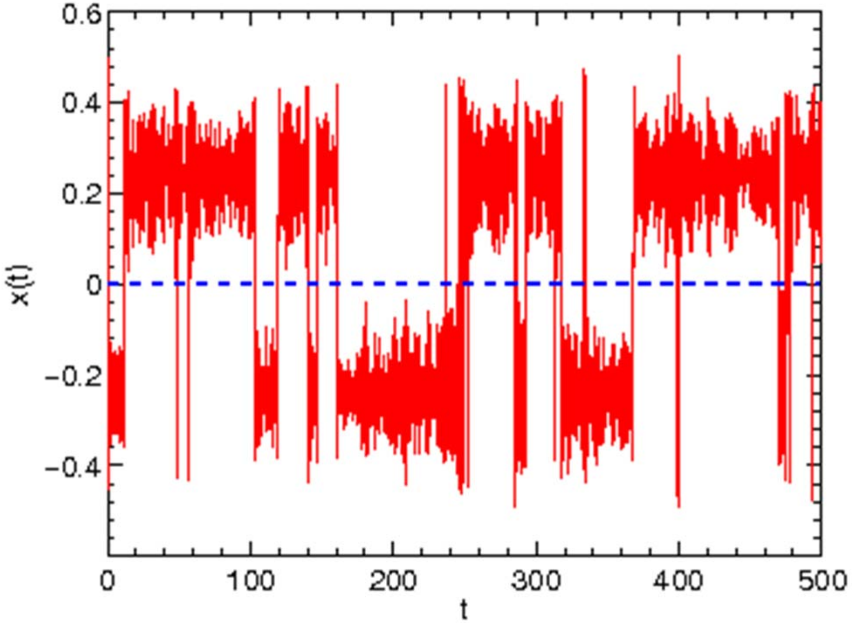
$$\Delta V = \frac{1}{4a}$$

Mpt(a) = ?









Task 3

Рівняння Ланжевена

$$x_n = x_{n-1} + f(x_{n-1})\Delta t + \sqrt{D\Delta t}\,\xi(t)$$

$$f(x) = -\frac{dV}{dx}$$

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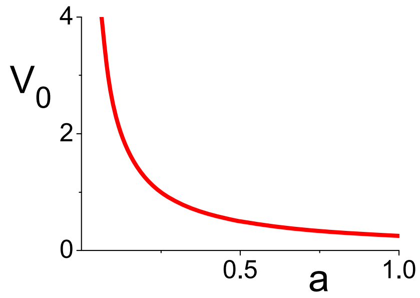
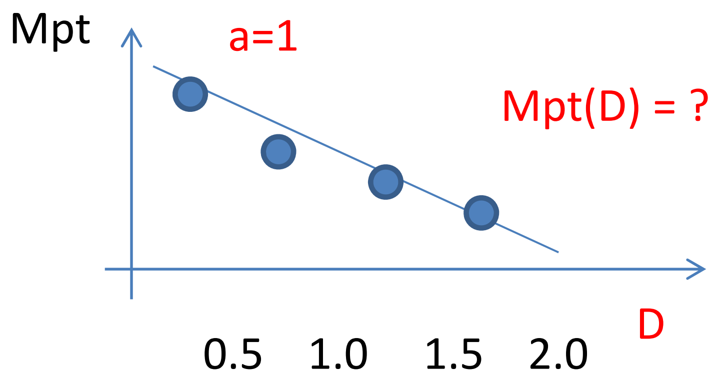
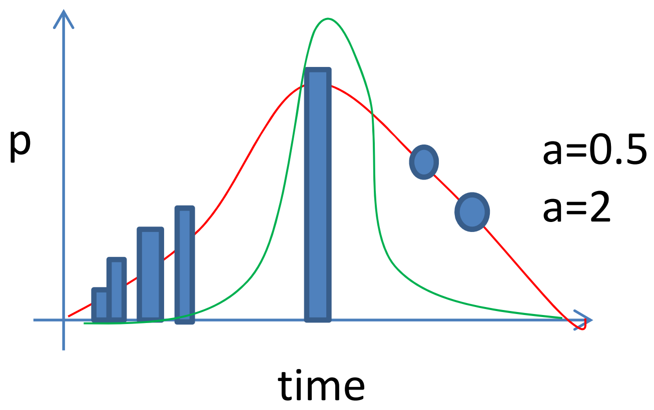
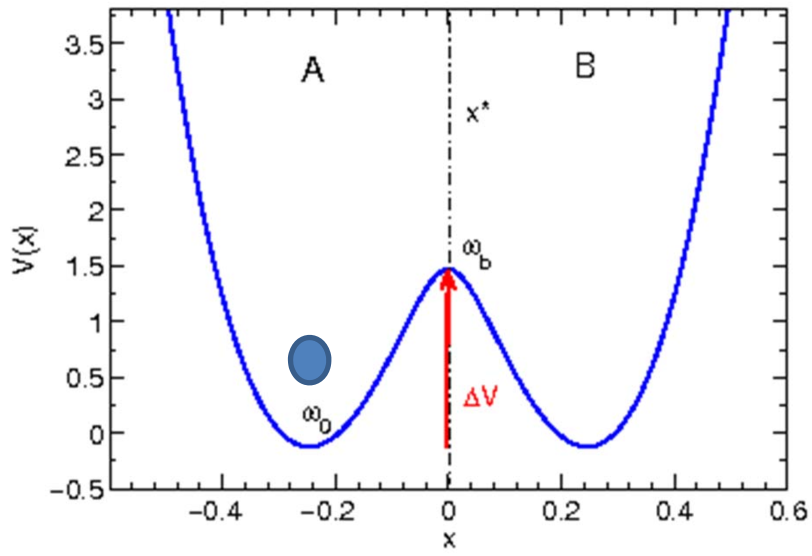
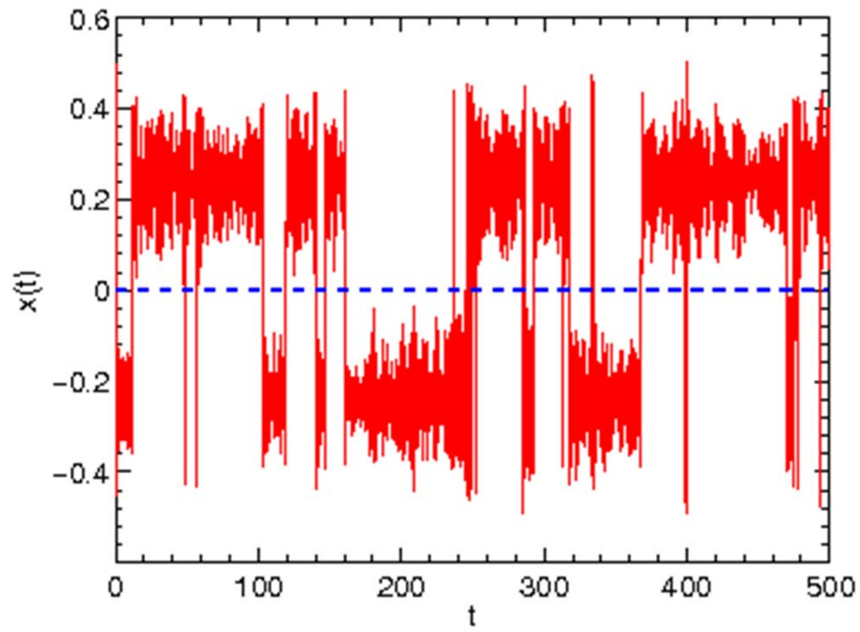


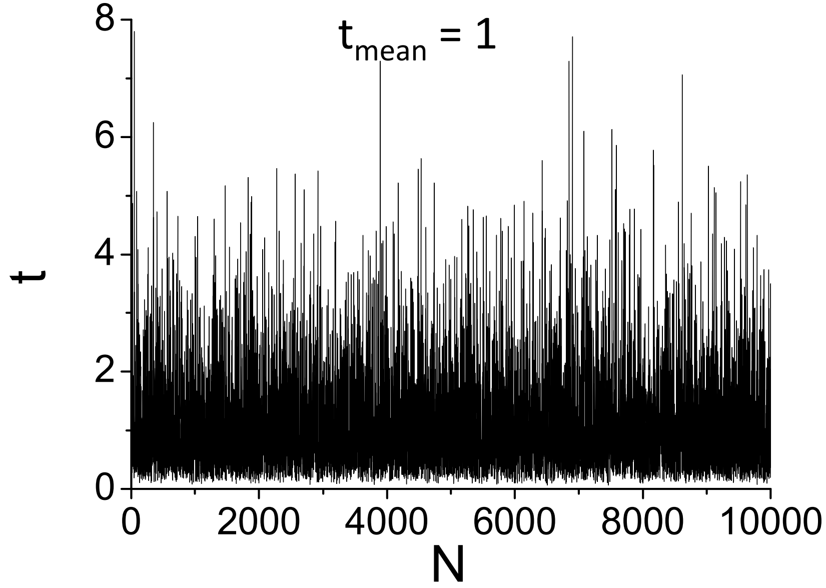


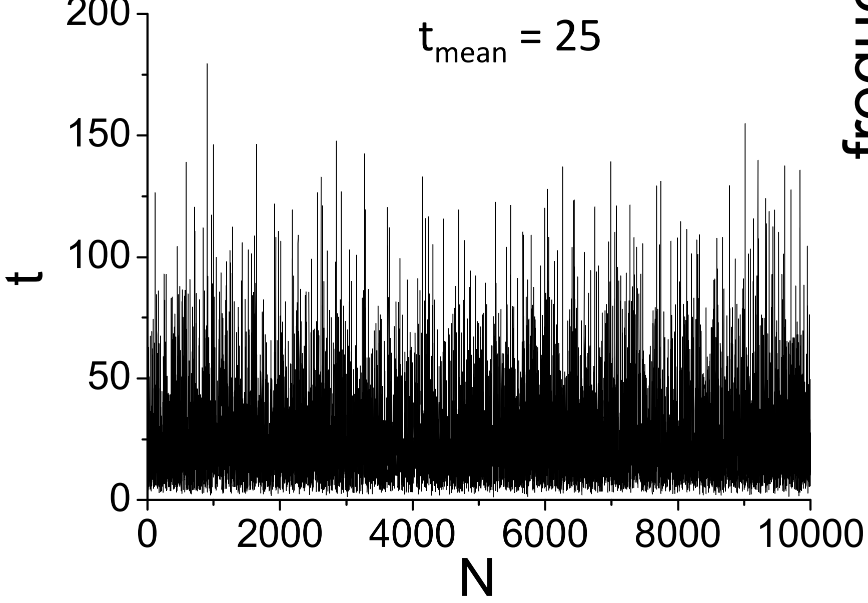


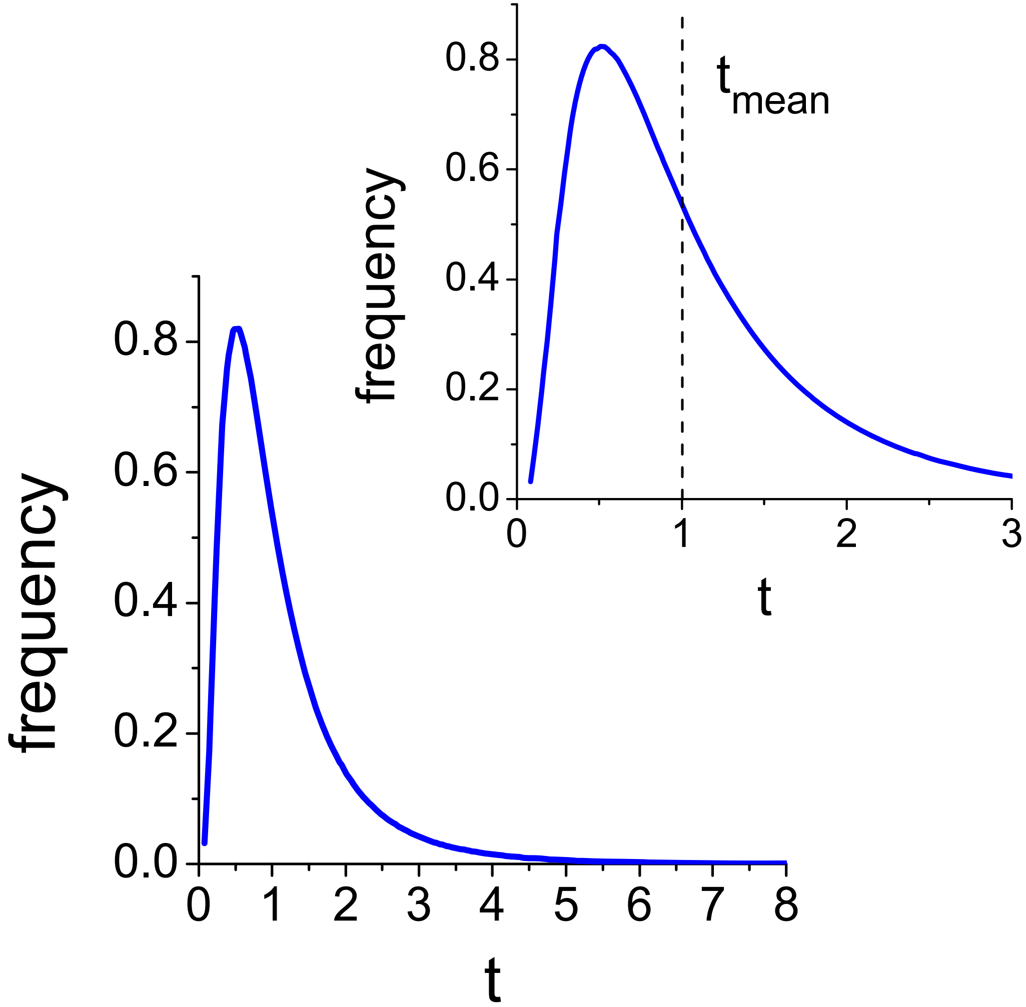




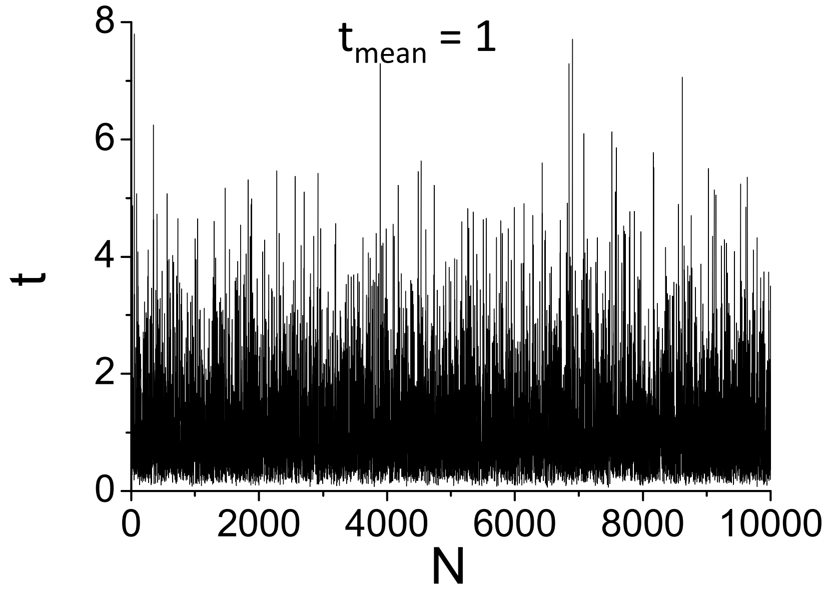
Рівняння Ланжевена

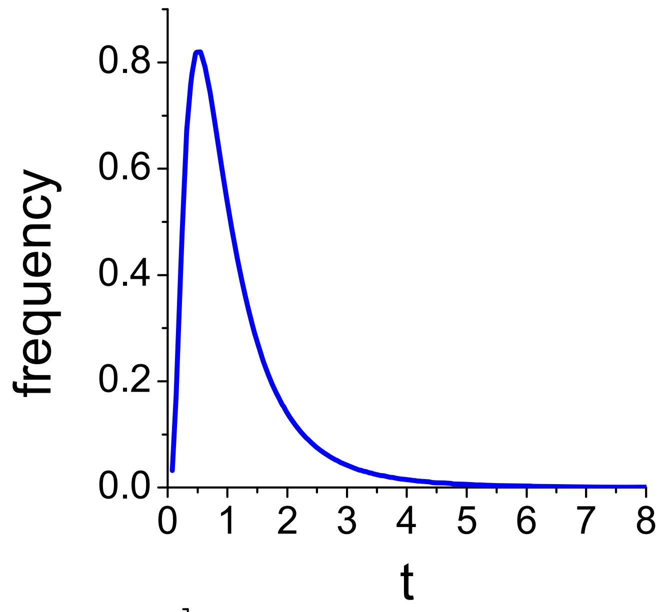


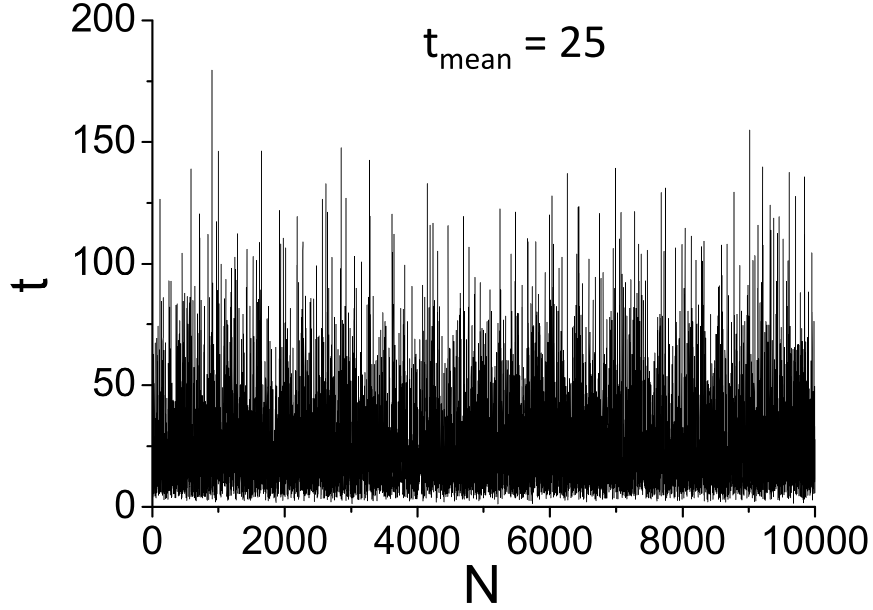


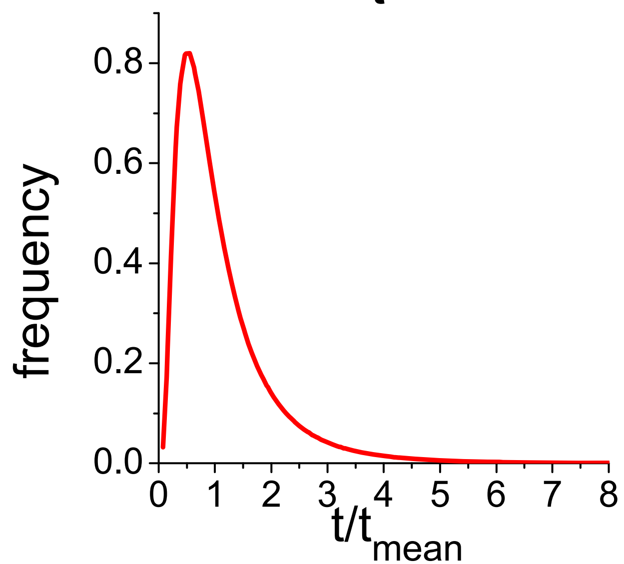


Рівняння Ланжевена

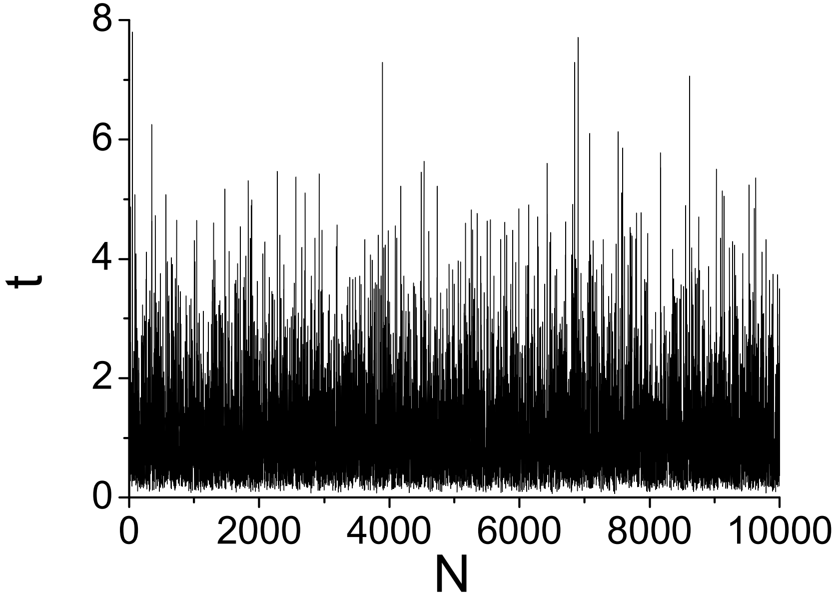




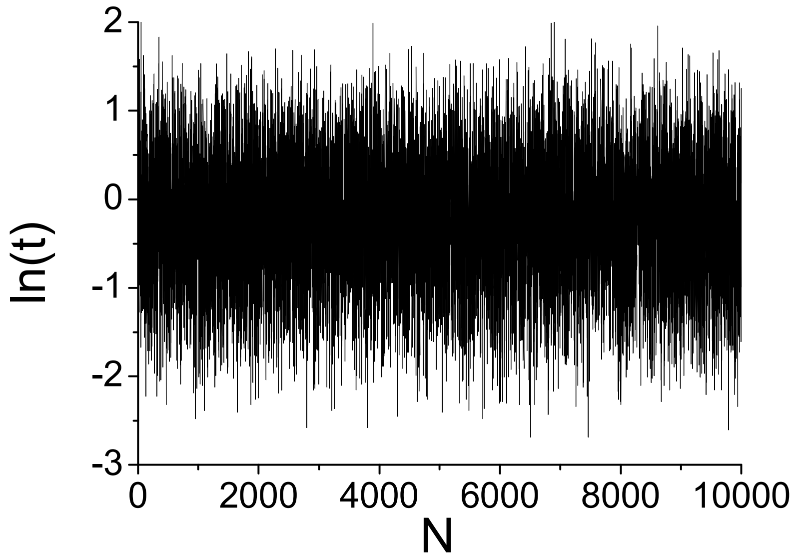




Рівняння Ланжевена



t = ln(t)



Рівняння Ланжевена

Гаусовий розподіл $$f_G = \frac{1}{\sigma\sqrt{2\pi}} exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Лог-нормальний розподіл $$f_{lg} = \frac{1}{y\sigma\sqrt{2\pi}} exp\left(-\frac{\left(\ln(y/\mu)\right)^2}{2\sigma^2}\right)$$

$$f_G \to f_{lg}: \quad x = \ln(y); \quad f_G(x)dx = f_{lg}(y)dy; \quad f_{lg}(y) = f_G(x)\frac{dx}{dy};$$

$$\frac{dx}{dy} = \frac{1}{y}; \quad f_{lg}(y) = \frac{1}{y\sigma\sqrt{2\pi}} exp\left(-\frac{(\ln(y)-\ln(\mu))^2}{2\sigma^2}\right)$$