

Комп'ютерне моделювання задач прикладної математики

Дифузія невзаємодіючих частинок. Рівняння Ланжевена

Лабораторна робота 1

$$i = 1 \dots N$$

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

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

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

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

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

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

```
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);
}
```

$$i = 1 \dots N$$

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

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

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

```
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;
```

```
Fprintf( t, Delta)
```

```
t_write+=dt_write
```

```
}
```

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

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

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

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

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

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

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

```
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```

Рівняння Ланжевена

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

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

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

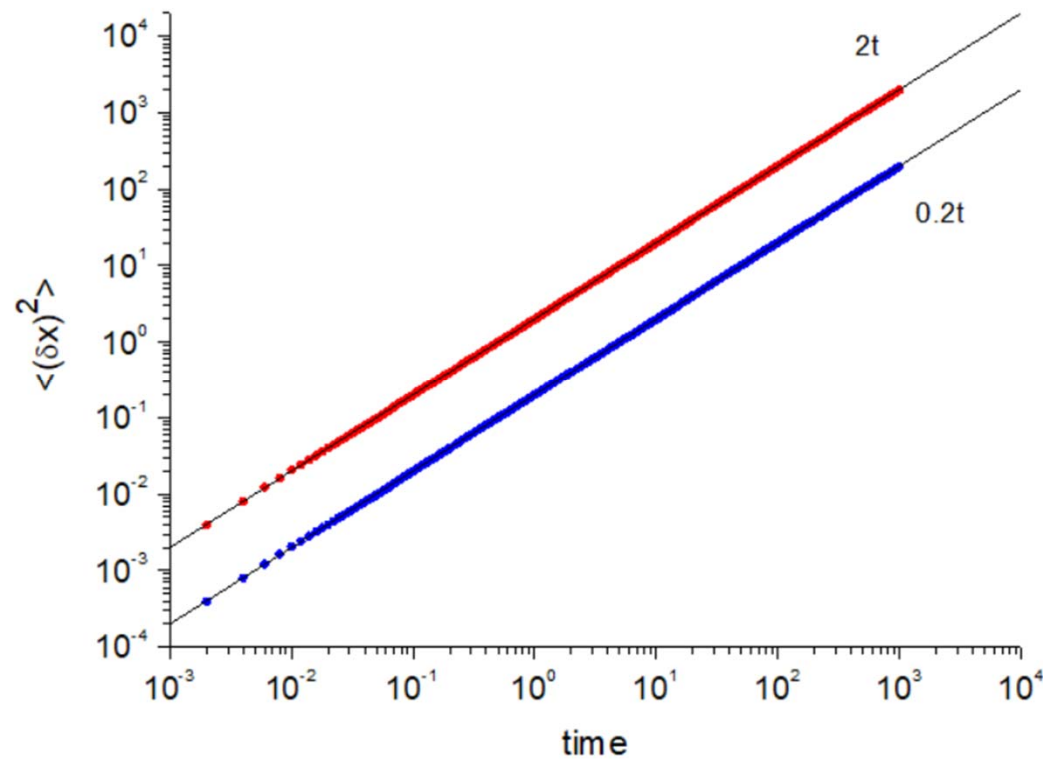
```
double ksi()  
{  
  double p1=rand()/(RAND_MAX+1.0);  
  double p2=rand()/(RAND_MAX+1.0); if (!p1)  
    p1=1e-10;  
  return sqrt(-2*log(p1))*sin(2.0*pi*p2);  
}
```

Рівняння Ланжевена

Task 1

$$f(x) = 0$$

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



$$N=10^4$$

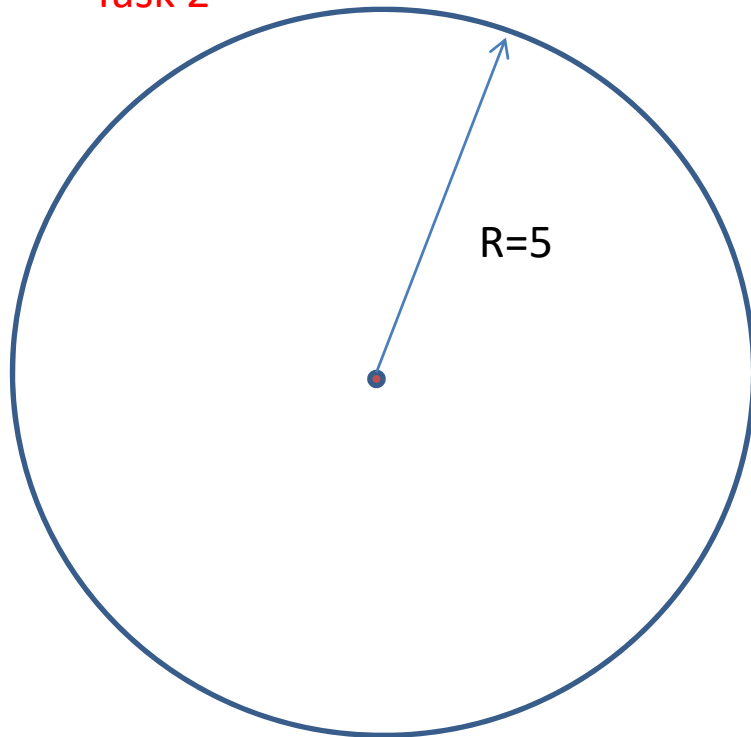
$$\Delta t = 0.002$$

Рівняння Ланжевена

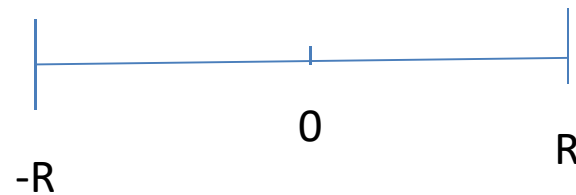
$$f(x) = 0$$

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

Task 2

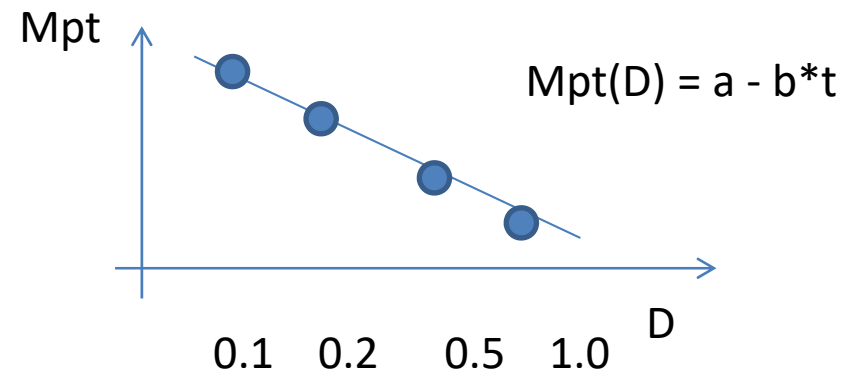
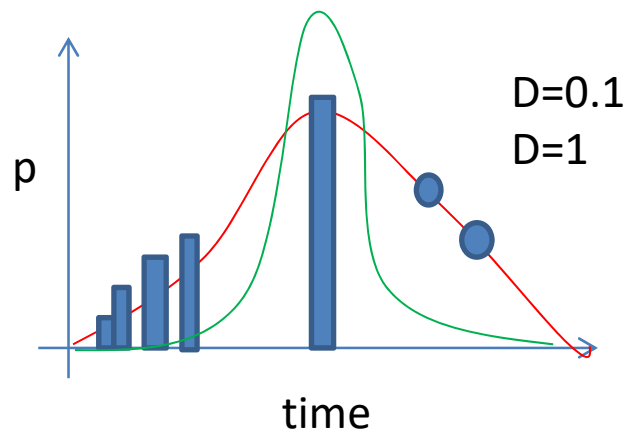


Target time



$$N=10^4$$

$$\Delta t = 0.002$$



Task 3

Рівняння Ланжевена

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

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

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

