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Diffusion example, simulation of a random walk

Try changing these variables, number of particles, step size, number of steps

$Number\_of\_particles := 2200$ $Step\_size := 5$ $Number\_of\_steps := 1000$

$j := 0 .. Number\_of\_particles$

$part_j := 0$ $drift := 0$ add some drift

Let the computer roll the dice

```
Simulate(part) := | delta ← Step_size
                  | for  j ∈ 0 .. Number_of_particles
                  |   | for  i ∈ 1 .. Number_of_steps
                  |   |   | sign ← 1   if  rnd(1) > 0.5
                  |   |   | sign ← −1   otherwise
                  |   |   | part_j ← part_j + sign·Step_size + drift
                  |   | v_j ← part_j
                  | return  v
```

This is a simple program, we have an array of numbers that we randomly increase or decrese by a Step_size increment for each step. We perform this operation until we reach the number of steps value. It is two loops, one to do the stepping for each particle and, an overall loop to march through an "ensemble" of particles.

$tt := Simulate(part)$

tt is the array of numbers

$m := Number\_of\_particles - 50$

tt =

	0
0	20
1	-200
2	390
3	60
4	-110
5	260
6	180
7	70

calculate the mean

$$\mu_{tt} := \frac{1}{m} \cdot \sum_{j=1}^{m} tt_j$$

calculate the standard deviation

$$sig_{tt} := \sqrt{\frac{1}{m} \cdot \sum_{j=1}^{m} \left(tt_j - \mu_{tt}\right)^2}$$

$\mu_{tt} = 2.391$ this mean stays around zero

$sig_{tt} = 158.888$ this standard deviation grows

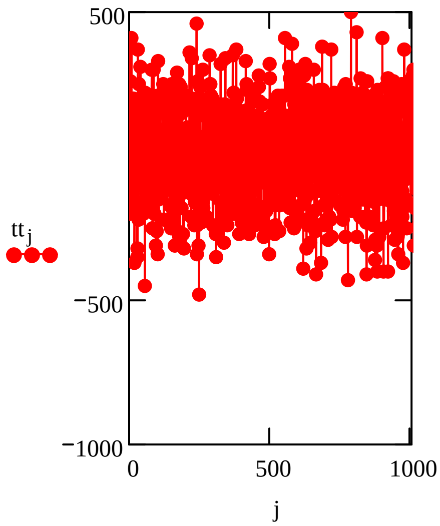
$\alpha := -500, -480 .. 500 + drift \cdot Number\_of\_steps$

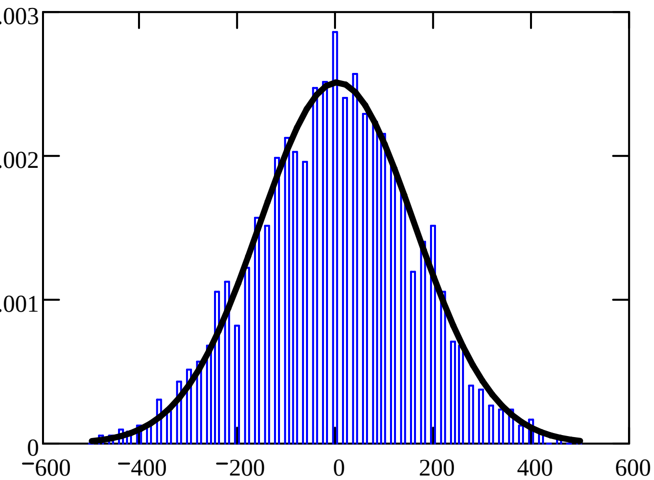
$$P(z,\alpha,\Delta) := \frac{1}{\Delta \cdot m} \cdot \sum_{i=0}^{m} if\left[\left(\alpha - \frac{\Delta}{2}\right) < z_i \le \left(\alpha + \frac{\Delta}{2}\right), 1, 0\right]$$

theoretically we get:

$$P_{Gauss}(z,\mu,\sigma) := \frac{1}{\sigma \cdot \sqrt{2 \cdot \pi}} \cdot e^{-\frac{(z-\mu)^2}{2 \cdot \sigma^2}}$$

Shape is Gaussian





Does Diffusion Velocity make sense?

Diffusion constant for a small molecule in water is 10^{-5} cm^2/s

$$D_{const} := 10^{-5}$$

Diffusion constant for a small molecule in air is 10^{-1} cm^2/s

$distance\_diffuse := 1 \cdot 10^{-6}$ 1 micron

$$time\_diffuse(x) := \frac{x^2}{2 \cdot D_{const}} \cdot 100^2$$

$time\_diffuse(distance\_diffuse) = 5 \times 10^{-4}$ seconds

$distance\_diffuse2 := 10 \cdot 10^{-6}$ 10 um

$time\_diffuse(distance\_diffuse2) = 0.05$ seconds

$distance\_diffuse3 := 1 \cdot 10^{-2}$ 1 cm

$time\_diffuse(distance\_diffuse3) = 5 \times 10^{4}$ seconds about 14 hours