

# Excercise 1

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Molecular Simulation

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## 1 Task 1

Given a square with length  $l$  and a circle lying within that circle with radius  $r = \frac{l}{2}$  we can define the surface ratio  $r_s$  as

$$r_s = \frac{\pi r^2}{(2r)^2} \quad (1)$$

re-arranging terms yields in an expression for

$$\pi = 4r_s \quad (2)$$

The surface ration  $r_s$  can easily be approximated using Monte Carlo methods. First you draw  $N$  uniformly distributed random samples within the square. Then the surface ratio is approximated by the quotient of number of samples that lie within the circle  $N_{in}$  and the total number of samples generated  $N$ .

$$r_s \approx \frac{N_{in}}{N} \quad (3)$$

$$r_s = \frac{\pi r^2}{l^2} r a t^2 \quad (4)$$