Calculation of n[r] for an ideal gas

- n[r] represents the average number of particles found at a distance d
  $r \leq d \leq r + \Delta r$ of particle i

- For an ideal gas, the position of all particles is independent

- Theoretical result

- Monte Carlo code

- Compare the Monte Carlo result (histogram) with the theoretical result

- Plot the ratio of the Monte Carlo result (histogram) over the theoretical result

  $$g[r] \equiv \frac{n_{MC}[r]}{n_{ideal\_gas}[r]}.$$ Should be 1, by construction. This is a check of your MC code!

- When successful, proceed to implement the Boltzmann probability distribution via the Metropolis algorithm (exercice 5).

Theoretical result (N particles, 2 D box of length L, density $= N / L^2$)

the probability that any particle is located inside a surface ΔS is

$$p = \Delta S / S = \Delta S / L^2$$

The expectation value of the number of particles located inside ΔS is

$$p N = \Delta S \; N / L^2 = \Delta S \; \rho$$

The area ΔS around particle i , at a distance $r \leq d \leq r + \Delta r$ is

$\Delta S = 2 \pi r \Delta r$ $\qquad$ $\Delta r \equiv$ bin size of the histogram

The theoretical expectation of the number of particles found at $d \in \{ r , r + \Delta r \}$

of any particle is

$$n[r] = \Delta S \; \rho = \rho \; 2 \pi r \Delta r = (N / L^2) \; 2 \pi r \Delta r$$

As an example, take $N = 1000$, $L = 10$, $\Delta r = 0.1$

We have then $n[r] = 2 \pi r$

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With[{L = 10}, Plot[2 π r, {r, 0, L / 2}, AxesLabel → {r, n[r]}]]
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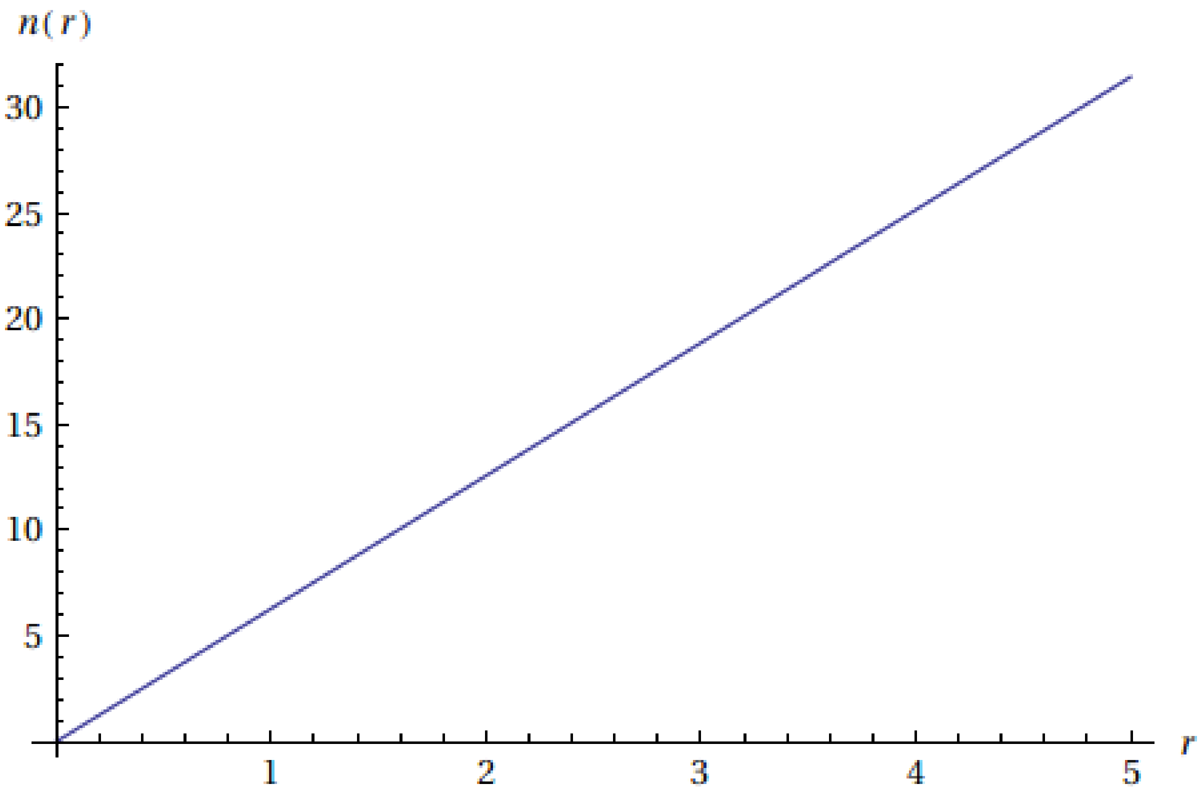

Write a MC code where $N = 1000$ particles are uniformly distributed inside a 2 d box of size $L = 10$

Compute all pair distances r_{ij} $\{i, 1, N-1\}$, $\{j, i+1, N\}$ and accumulate the value r_{ij} (increment of 1 in the counts of both particles) at bin number $r_{ij} / \Delta r$

- All N particles are identical, so a common count is enough. Just accumulate 1 in both bins of particles $\{i$ and $j\}$ $\rightarrow$ increment by 2
- Properly normalize the histogram dividing by $N \times$ Nsamples
- The pair distances r_{ij} must be computed as the smallest distance between the images of particles i and j
- Plot together the resulting histogram and the theoretical value $n[r] = 2\pi r$