Kinetic Monte Carlo Review Notes

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Monte Carlo Methods

- Solve complex problems using random sampling from a probablity distribution (i.e. stochastic description).
- Useful to evolve a physical system to a new state from an esemble of potential future states.

Integrating a function MC sampling

- If we want to evaluate the integral of a function over some domain we can numerically approximate this using the midpoint rule:

$$\int_a^b f(x)dx = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i) \tag{1}$$

- There is an alternative way to do this using probablity theory to determine the expectation value of a function $f(x)$ for random variable x:

$$\int_a^b p(x)f(x)dx = \frac{b-a}{N}\sum_{i=1}^{N} f(x_i) \tag{2}$$

  where $p(x)$ is a uniform probablity distribution over the interval $[a, b]$.

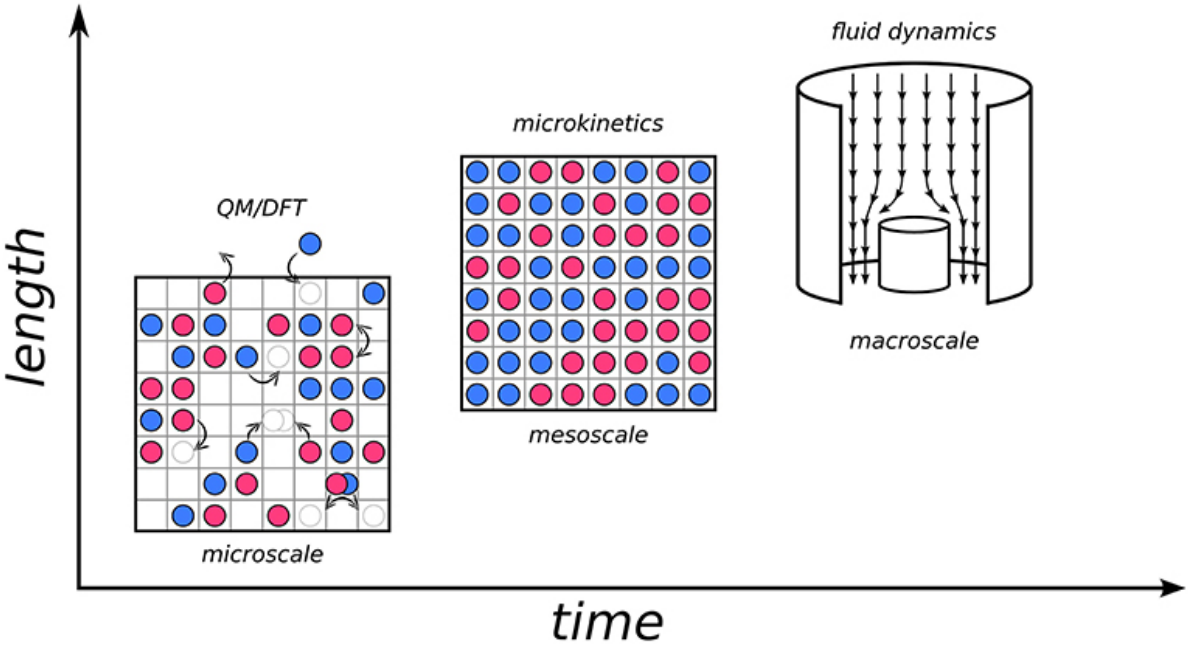

Figure 1: Monte Carlo methods Andersen, Panosetti, and Reuter (2019)

- The difference between numerically evaluating Equation 1 and Equation 2, is that Equation 1 is evaluated over a grid of points and Equation 2 is randomly sampled points.
- The error of MC integration is $\propto \frac{1}{\sqrt{N}}$ as a result of central limit theorem

Example integrating a function using MC sampling[1]

Example integrating a function using MC sampling

Backmatter

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[1] A more detailed notebook implementing the code can be viewed here

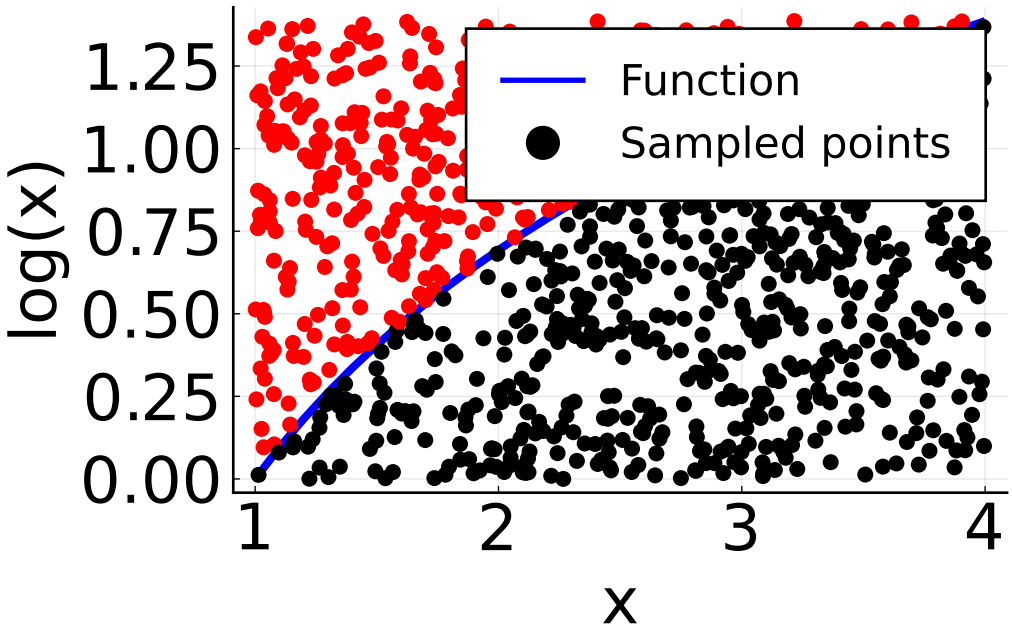

Figure 2: Random sampled points from uniform distribution over the interval $[1, 4]$. The black points are those that are accepted.

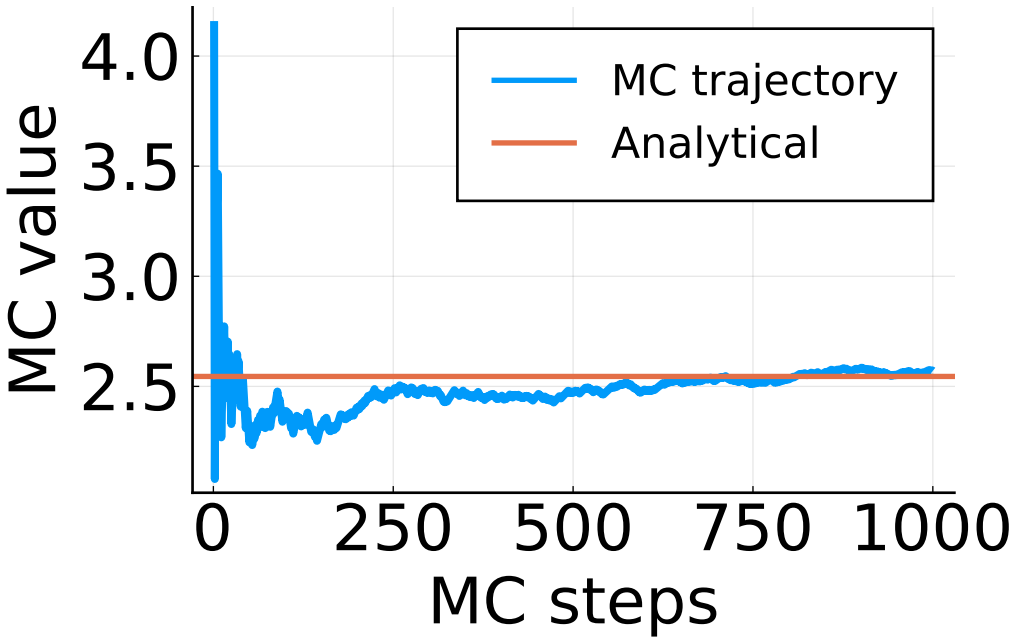

Figure 3: Integration of $log(x)$ using MC.

> **Note**
>
> This presentation can be viewed online at https://stefanbringuier.github.io/KMCNotes. A report formated PDF of this presentation can be downloaded here.

> **Tip**
>
> To export `revealjs` presentations to pdf, press 'e' then 'ctrl-p' 'save as pdf'

References & footnotes

Andersen, Mie, Chiara Panosetti, and Karsten Reuter. 2019. "A Practical Guide to Surface Kinetic Monte Carlo Simulations." *Frontiers in Chemistry* 7. https://doi.org/10.3389/fchem.2019.00202.