Not for students who get < 10 ECTS for the course

Computational Physics – Exercise 7: Diffusion equation

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Exercise 1

- Use the 2nd-order product formula algorithm $e^{tH} \approx (e^{tA/2m} e^{tB/m} e^{tA/2m})^m$ to solve the one-dimensional diffusion equation. Perform simulations for the set of parameters:
  - $D = 1$ (only fixes the "scale")
  - $L = 1001$
  - $\Delta = 0.1$
  - $\tau = 0.001$
  - $m = 10000$

$$\left\langle x^p(t) \right\rangle = \frac{\int_0^{L\Delta} x^p N(x,t)dx}{\int_0^{L\Delta} N(x,t)dx} \approx \Delta^p \frac{\sum_{i=1}^{L} (i-i_0)^p \Phi_i(t)}{\sum_{i=1}^{L} \Phi_i(t)}$$

- For two different initial conditions:

$$\Phi_i(t=0) = \begin{cases} 1 & i = i_0 \equiv (L+1)/2 \\ 0 & i \neq i_0 \equiv (L+1)/2 \end{cases} \quad \text{and} \quad \Phi_i(t=0) = \begin{cases} 1 & i = 1 \\ 0 & i \neq 1 \end{cases}$$

- Plot $\Delta^{-2}\left(\left\langle x^2(t)\right\rangle - \left\langle x(t)\right\rangle^2\right)$ as a function of *t*
- Interpret the results!

Exercise 2: Diffusion comparison with random walk

- $N = 10000$ particles all start at the center $(L+1)/2$ of the system, making random walks as described earlier. $N_i(t)$ is the number of walkers at site i and discrete time t
- $L = 1001$
- $t = 0, 1, 2, \ldots, 10$

$$\left\langle x^p(t) \right\rangle = \frac{\sum_{i=1}^{L} (i - i_0)^p N_i(t)}{\sum_{i=1}^{L} N_i(t)}$$

- Plot $\left\langle x^2(t) \right\rangle - \left\langle x(t) \right\rangle^2$ as a function of t
- Compare with results of diffusion equation

$$\Delta = 0.1, \quad \tau = 0.001 \quad \Rightarrow D = \Delta^2 / 2\tau = 5$$

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Report

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- Filename: Report_7_Surname1_Surname2.pdf, where Surname1 < Surname2 (alphabetical order).
  Example: Report_7_Jin_Willsch.pdf (Do not use “umlauts” or any other special characters in the names)
- Content of the report:
  - Names + matricle numbers + e-mail addresses + title
  - Introduction: describe briefly the problem you are modeling and simulating (write in complete sentences)
  - Simulation model and method: describe briefly the model and simulation method (write in complete sentences)
  - Simulation results: show figures (use grids, with figure captions !) depicting the simulation results. Give a brief description of the results (write in complete sentences)
  - Discussion: summarize your findings
  - Appendix: Include the listing of the program

Due date: 10 AM, June 26, 2023