Computational Physics 2023

Sommersemester, 3th April, 2023 – 14th Juli, 2023

1) Introduction
2) Numbers and errors
3) Differentiation and integration
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5) Molecular dynamics simulations
6) **Partial differential equations**
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11) Monte Carlo (MC) Simulations
12) Perkolation
13) Stochastic Dynamics

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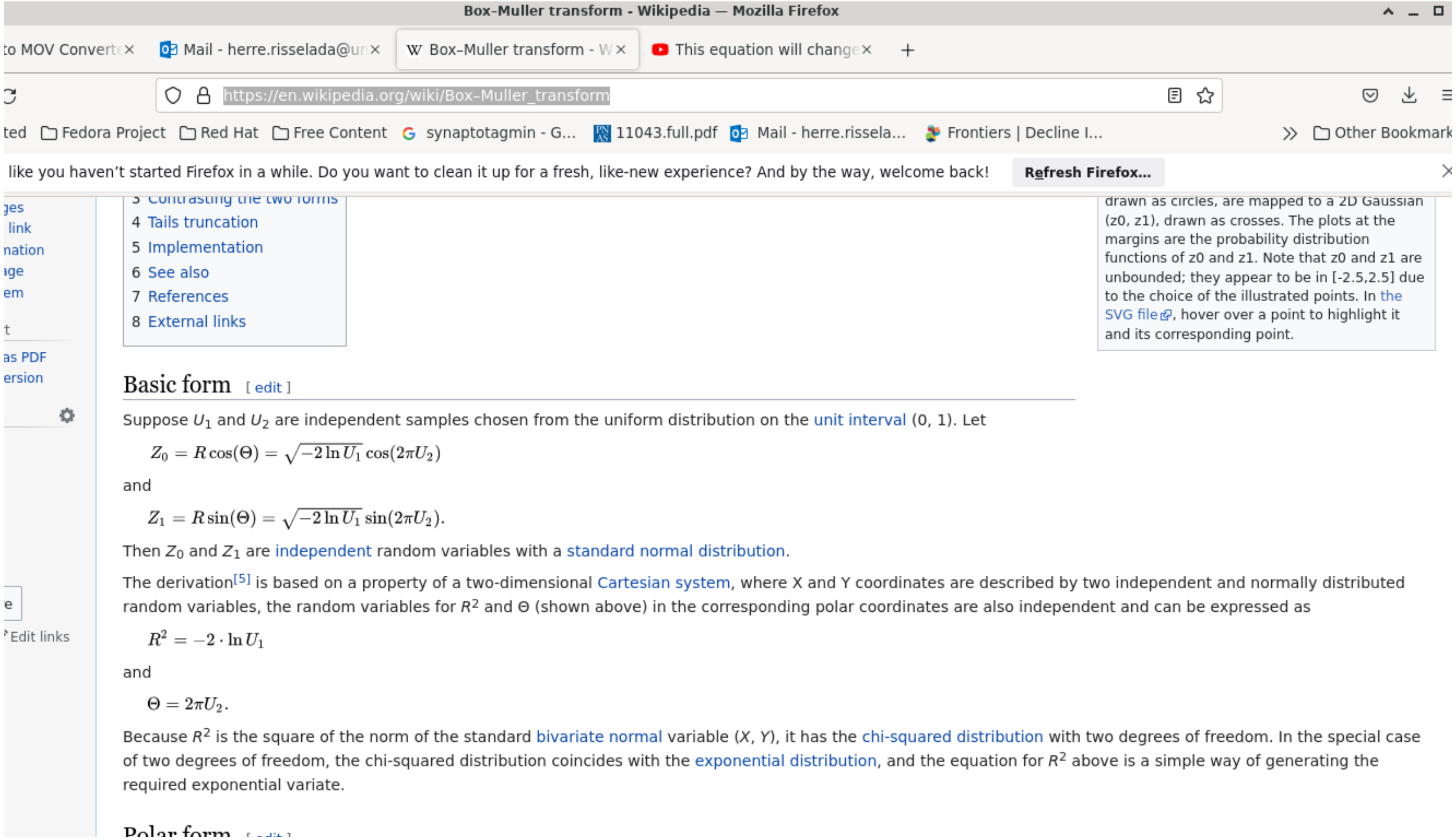
Setting up simulations

$$v_{i,\alpha} = \sqrt{\frac{k_\mathrm{B}T}{m_i}}\,\mathcal{N}(0,1)\,, \quad \alpha \in \{x, y, z\}\,,$$



Box-Muller transform - Wikipedia — Mozilla Firefox

https://en.wikipedia.org/wiki/Box-Muller_transform

drawn as circles, are mapped to a 2D Gaussian (z0, z1), drawn as crosses. The plots at the margins are the probability distribution functions of z0 and z1. Note that z0 and z1 are unbounded; they appear to be in [-2.5,2.5] due to the choice of the illustrated points. In the SVG file, hover over a point to highlight it and its corresponding point.

Basic form [edit]

Suppose U_1 and U_2 are independent samples chosen from the uniform distribution on the unit interval (0, 1). Let

$$Z_0 = R\cos(\Theta) = \sqrt{-2\ln U_1}\cos(2\pi U_2)$$

and

$$Z_1 = R\sin(\Theta) = \sqrt{-2\ln U_1}\sin(2\pi U_2).$$

Then Z_0 and Z_1 are independent random variables with a standard normal distribution.

The derivation[5] is based on a property of a two-dimensional Cartesian system, where X and Y coordinates are described by two independent and normally distributed random variables, the random variables for R^2 and Θ (shown above) in the corresponding polar coordinates are also independent and can be expressed as

$$R^2 = -2\cdot\ln U_1$$

and

$$\Theta = 2\pi U_2.$$

Because R^2 is the square of the norm of the standard bivariate normal variable (X, Y), it has the chi-squared distribution with two degrees of freedom. In the special case of two degrees of freedom, the chi-squared distribution coincides with the exponential distribution, and the equation for R^2 above is a simple way of generating the required exponential variate.

Discrete Poisson equation

https://en.wikipedia.org/wiki/Discrete_Poisson_equation

$$(\nabla^2 u)_{ij} = \frac{1}{\Delta x^2}(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}) = g_{ij}$$

$$A\mathbf{u} = \mathbf{b}$$

$$\mathbf{u} = [\,u_{11}, u_{21}, \ldots, u_{m1}, u_{12}, u_{22}, \ldots, u_{m2}, \ldots, u_{mn}\,]^{\mathsf{T}}$$

$$\mathbf{b} = -\Delta x^2 [\,g_{11}, g_{21}, \ldots, g_{m1}, g_{12}, g_{22}, \ldots, g_{m2}, \ldots, g_{mn}\,]^{\mathsf{T}}.$$

$$A = \begin{bmatrix} D & -I & 0 & 0 & 0 & \cdots & 0 \\ -I & D & -I & 0 & 0 & \cdots & 0 \\ 0 & -I & D & -I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -I & D & -I & 0 \\ 0 & \cdots & \cdots & 0 & -I & D & -I \\ 0 & \cdots & \cdots & \cdots & 0 & -I & D \end{bmatrix}, \qquad D = \begin{bmatrix} 4 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 4 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 4 & -1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 4 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 4 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 4 \end{bmatrix},$$

Discrete Poisson equation

https://en.wikipedia.org/wiki/Discrete_Poisson_equation

$$A = \begin{bmatrix} D & -I & 0 & 0 & 0 & \cdots & 0 \\ -I & D & -I & 0 & 0 & \cdots & 0 \\ 0 & -I & D & -I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -I & D & -I & 0 \\ 0 & \cdots & \cdots & 0 & -I & D & -I \\ 0 & \cdots & \cdots & \cdots & 0 & -I & D \end{bmatrix},$$

$$D = \begin{bmatrix} 4 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 4 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 4 & -1 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 4 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & -1 & 4 & -1 \\ 0 & \cdots & \cdots & \cdots & 0 & -1 & 4 \end{bmatrix},$$

m=5,n=5

$$A = \left[\begin{array}{ccc|ccc|ccc} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ \hline -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ \hline 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{array}\right]$$

$$D = \begin{bmatrix} 4 & -1 & 0 \\ -1 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}$$

$$-I = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

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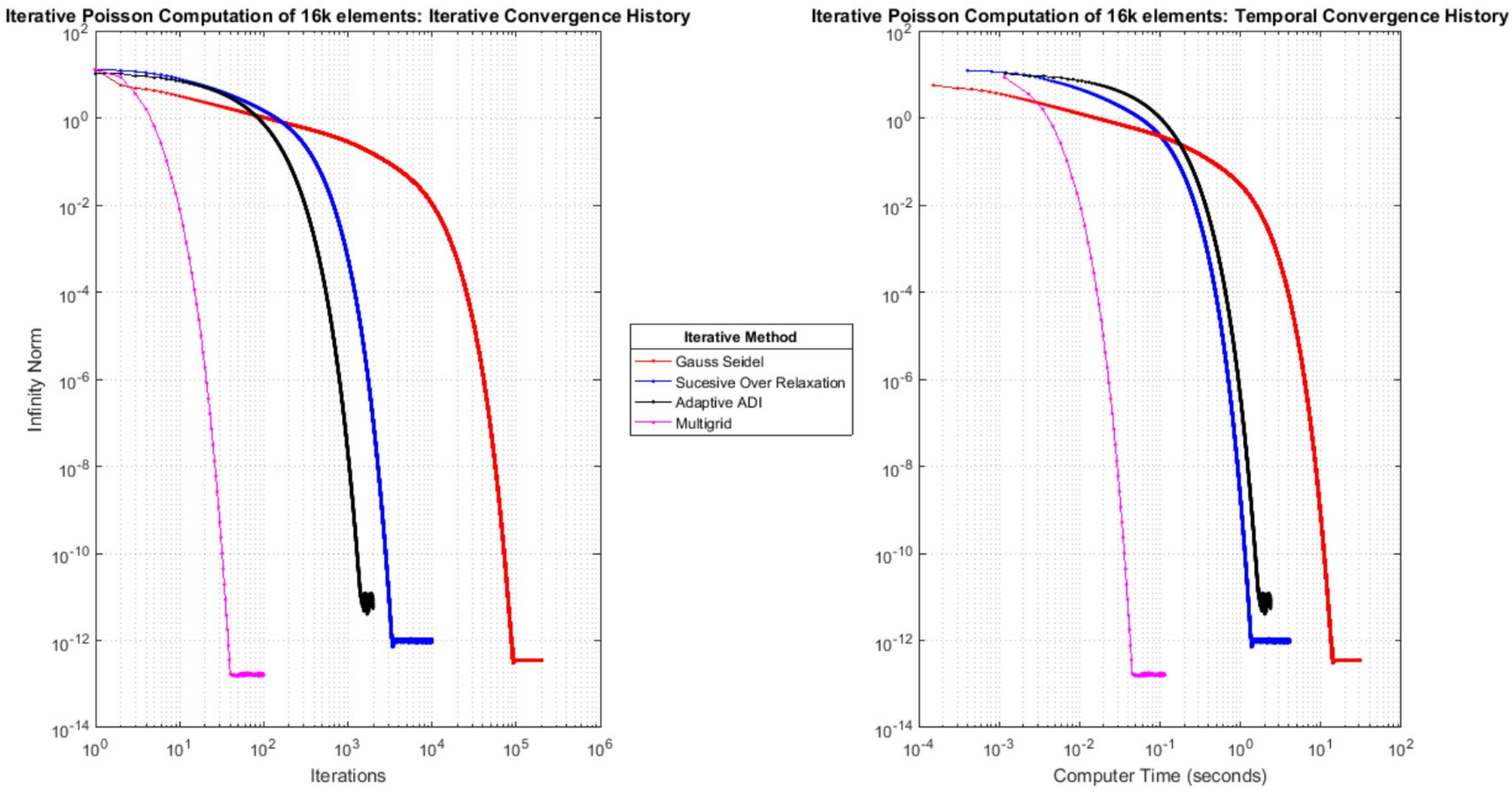
Discrete Poisson equation



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Schroedinger Equation

$$\mathbf{A}\cdot\mathbf{x} = \mathbf{M}\cdot\mathbf{y}$$

$$\mathbf{A}\!\cdot\!\mathbf{x} = \begin{pmatrix}
a_0 & -r_x & 0 & 0 & \cdots & 0 & -r_y & 0 & 0 & \cdots & 0 \\
-r_x & a_1 & -r_x & 0 & \cdots & & 0 & -r_y & 0 & \cdots & 0 \\
0 & -r_x & a_2 & -r_x & & & & & -r_y & & \\
0 & 0 & -r_x & \ddots & \ddots & & & & & \ddots & \\
\vdots & \vdots & & \ddots & & & & & & & \\
0 & & & & & & & & & & \\
-r_y & 0 & & & & & & & & & \\
0 & -r_y & & & & & & & & & \\
0 & 0 & -r_y & & & & & & & \ddots & \\
\vdots & \vdots & & \ddots & & & & & \ddots & \ddots & -r_x \\
0 & 0 & & & & & & & & -r_x & a_{(N-3)(N-1)}
\end{pmatrix}
\begin{pmatrix}
\psi_0^{n+1} \\ \psi_1^{n+1} \\ \psi_2^{n+1} \\ \\ \vdots \\ \\ \psi_k^{n+1} \\ \\ \vdots \\ \\ \psi_{(N-3)(N-1)}^{n+1}
\end{pmatrix}$$

$$r_x = -\frac{\Delta t}{2i(\Delta x)^2}\,, \quad r_y = -\frac{\Delta t}{2i(\Delta y)^2}\,.$$

$$a_{ij} = \left(1 + 2r_x + 2r_y + i\frac{\Delta t}{2}V_{i,j}^{n+1}\right)$$

$$b_{ij} = \left(1 - 2r_x - 2r_y - i\frac{\Delta t}{2}V_{i,j}^{n}\right)$$

$$\mathbf{b} = \mathbf{M}\!\cdot\!\mathbf{y} = \begin{pmatrix}
b_0 & r_x & 0 & 0 & \cdots & 0 & r_y & 0 & 0 & \cdots & 0 \\
r_x & b_1 & r_x & 0 & \cdots & & 0 & r_y & 0 & \cdots & 0 \\
0 & r_x & b_2 & r_x & & & & & r_y & & \\
0 & 0 & r_x & \ddots & \ddots & & & & & \ddots & \\
\vdots & \vdots & & \ddots & & & & & & & \\
0 & & & & & & & & & & \\
r_y & 0 & & & & & & & & & \\
0 & r_y & & & & & & & & & \\
0 & 0 & r_y & & & & & & & \ddots & \\
\vdots & \vdots & & \ddots & & & & & \ddots & \ddots & r_x \\
0 & 0 & & & & & & & & r_x & b_{(N-3)(N-1)}
\end{pmatrix}
\begin{pmatrix}
\psi_0^{n} \\ \psi_1^{n} \\ \psi_2^{n} \\ \\ \vdots \\ \\ \psi_k^{n} \\ \\ \vdots \\ \\ \psi_{(N-3)(N-1)}^{n}
\end{pmatrix}$$

Schroedinger Equation

$$\psi(x,y,t=0) = e^{-\frac{1}{2\sigma^2}\left[(x-x_0)^2+(y-y_0)^2\right]} \cdot e^{-ik(x-x_0)} .$$