Universität of Göttingen
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Methods of Computational Physics
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Sheet 6: Partial Differential Equations

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- **Modified diffusion equation – initial value problem**

  The Schrödinger equation in imaginary time, τ, takes the form

  $$-\frac{\partial \psi}{\partial \tau} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \tag{1}$$

  where $\Psi(x,\tau)$ denotes the particle's wavefunction and $V(x)$ is the external potential.

  $$V(x) = \frac{1}{2}m\omega^2\left[\frac{L}{\pi}\cos\left(\frac{\pi x}{L}\right)\right]^2 - E_T \tag{2}$$

  The potential, $V(x)$, is periodic with spatial period L. Therefore, we only consider the interval $[0:L]$ and apply periodic boundary conditions. In the following we rescale all lengths by $x_0^2 = \frac{\hbar}{m\omega}$ and all energies by $\hbar\omega$.

  a) Use the above length and energy scale to rewrite Equation 1 in a dimensionless form. There is a critical value of E_T^*, for which the norm of the wavefunction becomes independent of time, τ. Can you estimate E_T^* in the limit $L/x_0 \to \infty$ without calculation? Which limit does the wavefunction, $\Psi(x,\tau)$, adopt in the limit $\tau \to \infty$ (and $L/x_0 \to \infty$)?

  b) In the following, use $L = 20x_0$ and a discretize the spatial interval into $N_x = 200$ grid points. Use the initial condition $\Psi(x,\tau=0) = \delta(x - L/2)$ and propagate this initial wavefunction to $\tau_{\text{fin}} = 200$. For the following algorithms

     – forward Euler algorithm

     – Crank-Nicolson methods

     – pseudo-spectral technique

     describe your implementation of the algorithm, determine how small a time step $\Delta\tau = \frac{\tau_{\text{fin}}}{N_\tau - 1}$ is required for a stable and accurate solution, and estimate the critical value of E_T.

  c) Consider a smaller value, $L = 3x_0$ – what changes and how large is E_T?

- **Laplace equation – boundary value problem** Consider the two-dimensional Laplace equation

  $$\triangle\phi(x,y) = 0 \tag{3}$$

  in a quadratic domain of size $L \times L$. The potential ϕ vanishes on the boundary of the domains. There are N circular electrodes inside the domain with center (x_i, y_i) and radius r_i. The potential on the surface of the electrodes is set to V_i.

  a) Write a program that computes the potential, $\phi(x,y)$, using successive over relaxation (SOR). As stopping criterion assert that the error of the discretized Laplace equation is everywhere smaller than ϵ. Explain the method of successive over relaxation (SOR).

b) Construct a simple example, where you can (approximately) compute the potential with pencil and paper and verify your program by comparing your numerical data to the analytical solution. How does the solution depend on the spatial discretization? How does number of iterations depend on the over-relaxation parameter, α?

c) Consider the case of 4 electrodes in a unit domain, $L = 1$ with parameters

i	x_i	y_i	r_i	V_i
0	0.2	0.2	0.1	1
1	0.4	0.2	0.1	-1
2	0.7	0.3	0.1	1
3	0.5	0.8	0.1	1

Calculate the potential and plot it. Discuss a suitable choice of the spatial discretization and the convergence of the SOR algorithm.