

040692 PR Practical in numerical Astronomy

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One-dimensional diffusion equation

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One-dimensional diffusion equation:

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2} \quad (1)$$

Solve numerically the one-dimensional diffusion equation (1) in the box $-5 \leq x \leq +5$ using the Crank-Nicholson scheme with the initial condition set by the following equation:

$$\rho(x, t_0) = \exp\left(-\frac{x^2}{4Dt_0}\right) \quad (2)$$

For the diffusion coefficient, choose $D = 2$, the starting time $t_0 = 2.0$, and the number of grid cells in the x-direction $N = 100$. For the boundaries choose the Neumann and Dirichlet conditions. For the former, assume that the gradient of the density across the boundaries is equal to zero, while for the latter use the analytic solution of the form:

$$\rho(x, t) = \sqrt{\frac{t_0}{t_n}} \exp\left(-\frac{x^2}{4Dt}\right), \quad (3)$$

where t_n is the current time. To preserve accuracy, the maximum relative change in density every time step should not exceed 15 %, such that

$$\max_j \left(\frac{|\rho_j^{n+1} - \rho_j^n|}{\min(\rho_j^{n+1}, \rho_j^n)} \right) < 0.15.$$

The report contains:

- A brief introduction on the Crank-Nicholson method and the way you implemented it.
- The graphical representation of the solution for both boundary conditions at $t = 4.0$ and its comparison with the analytic solution.
- The total mass inside the computational domain as a function of time in the interval $t \in [2.0, 4.0]$ for each boundary condition. Provide an explanation for the observed trends.
- The analysis of the relative error between the numerical and exact solutions as a function of position x (also in the graphical form). Where are the minimum and maximum relative errors found (provide values)?

A brief introduction on the Crank-Nicholson method and the way you implemented it.

We divide the spatial domain into $N - 1$ intervals of length $\Delta x = \frac{L}{N-1}$, while using N equally distant grid points such that $x_i = (i - 1)N - \frac{L}{2}$ is the i -th centered grid point around zero, where L is total length. Equation (1) is defined in the domain $(x, t) \in [-5, 5] \times T$, where the temperature T is limited to $T \in [2, 4]$. For the initial time step we chose the Courant stability condition for the diffusion equation, which is given by $\Delta t \leq \frac{\Delta x^2}{2D}$. We adapt the notation such that $\rho(x_i, t_n) \equiv \rho_i^n$, where $i \in N$ and $t_n \in T$ (t_n depends on the accuracy setting), and write the Crank-Nicholson scheme as presented in the lecture notes as the sum of the forward-time centered-space (FTCS) and backward-time centered-space (BTCS) schemes

$$\frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} = \frac{D}{2} \left(\frac{\rho_{j+1}^{n+1} - 2\rho_j^{n+1} + \rho_{j-1}^{n+1}}{\Delta x^2} + \frac{\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n}{\Delta x^2} \right) + \mathcal{O}((\Delta x)^2). \quad (4)$$

Solving equation (4) for the new temperatures in terms of old temperatures we get

$$-\alpha\rho_{j-1}^{n+1} + (1 + 2\alpha)\rho_j^{n+1} - \alpha\rho_{j+1}^{n+1} = \underbrace{\alpha\rho_{j-1}^n + (1 - 2\alpha)\rho_j^n + \alpha\rho_{j+1}^n}_{=: u_j^n}, \quad (5)$$

where $\alpha = \frac{\Delta t D}{2(\Delta x)^2}$. Supposing a Dirichlet boundary conditions approach, we have to solve the following matrix equation

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ -\alpha & 1 + 2\alpha & -\alpha & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & -\alpha & 1 + 2\alpha & -\alpha \\ 0 & \dots & 0 & 0 & 1 \end{pmatrix}}_{\in \mathbb{R}^{N \times N}} \begin{pmatrix} \rho_0^{n+1} \\ \rho_1^{n+1} \\ \vdots \\ \vdots \\ \rho_N^{n+1} \end{pmatrix} = \begin{pmatrix} u_0^n \\ u_1^n \\ \vdots \\ \vdots \\ u_N^n \end{pmatrix}, \quad (6)$$

where the first and the last equation is the boundary condition with $u_0^n = \rho(x_0, t_n)$ and $u_N^n = \rho(x_N, t_n)$ as defined in equation (2).

For the Neumann boundary conditions (i.e. in our case for insulated boundaries) we need a special version of equation (5). We use therefor the fact that $\rho_{-1}^{n+1} \equiv \rho_1^{n+1}$ and get for the left boundary at $j = 0$

$$(1 + 2\alpha)\rho_0^{n+1} - 2\alpha\rho_1^{n+1} = \underbrace{(1 - 2\alpha)\rho_0^n + 2\alpha\rho_1^n}_{=: u_0^n}. \quad (7)$$

For the right boundary we use the fact that $\rho_{N-1}^{n+1} \equiv \rho_{N+1}^{n+1}$ at $j = N$ and get

$$(1 + 2\alpha)\rho_{N-1}^{n+1} - 2\alpha\rho_N^{n+1} = \underbrace{(1 - 2\alpha)\rho_N^n + 2\alpha\rho_{N-1}^n}_{=: u_N^n}. \quad (8)$$

Thus for Neumann boundary conditions, where

$$\frac{\partial \rho(x_0, t)}{\partial x} = 0 \quad \text{and} \quad \frac{\partial \rho(x_N, t)}{\partial x} = 0, \quad (9)$$

we have to solve the following matrix equation:

$$\underbrace{\begin{pmatrix} 1+2\alpha & -2\alpha & 0 & \dots & 0 \\ -\alpha & 1+2\alpha & -\alpha & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & -\alpha & 1+2\alpha & -\alpha \\ 0 & \dots & 0 & -2\alpha & 1+2\alpha \end{pmatrix}}_{\in \mathbb{R}^{N \times N}} \begin{pmatrix} \rho_0^{n+1} \\ \rho_2^{n+1} \\ \vdots \\ \vdots \\ \rho_{N-1}^{n+1} \\ \rho_N^{n+1} \end{pmatrix} = \begin{pmatrix} u_0^n \\ u_1^n \\ \vdots \\ \vdots \\ u_{N-1}^n \\ u_N^n \end{pmatrix}, \quad (10)$$

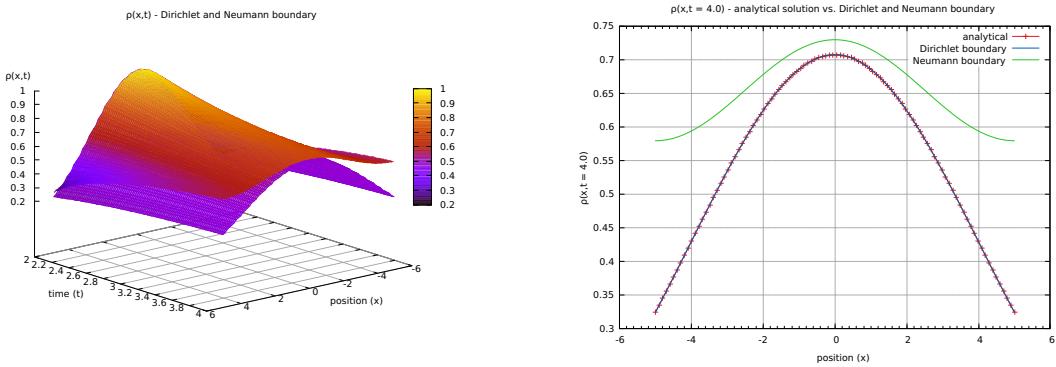
In opposite to the lecture notes we reformulate the linear system in such a way that the boundary specifications are included in the linear system and do not need to be updated separately. We further use the centered difference to approximate $\frac{\partial \rho(x_0, t)}{\partial x}$ and $\frac{\partial \rho(x_N, t)}{\partial x}$ (instead of forward or backward difference to represent the Neumann boundary condition at the left and the right end of the domain), by constructing the so-called "false points" such that

$$\frac{\partial \rho(x_0, t_{n+1})}{\partial x} = \frac{\rho_1^{n+1} - \rho_{-1}^{n+1}}{2\Delta x} + \mathcal{O}(\Delta x^2) = 0 \text{ and } \frac{\partial \rho(x_N, t_{n+1})}{\partial x} = \frac{\rho_{N-1}^{n+1} - \rho_{N+1}^{n+1}}{2\Delta x} + \mathcal{O}(\Delta x^2) = 0. \quad (11)$$

However, since both linear systems have a tridiagonal structure we can use the Thomas algorithm to solve the system for every time step t_n .

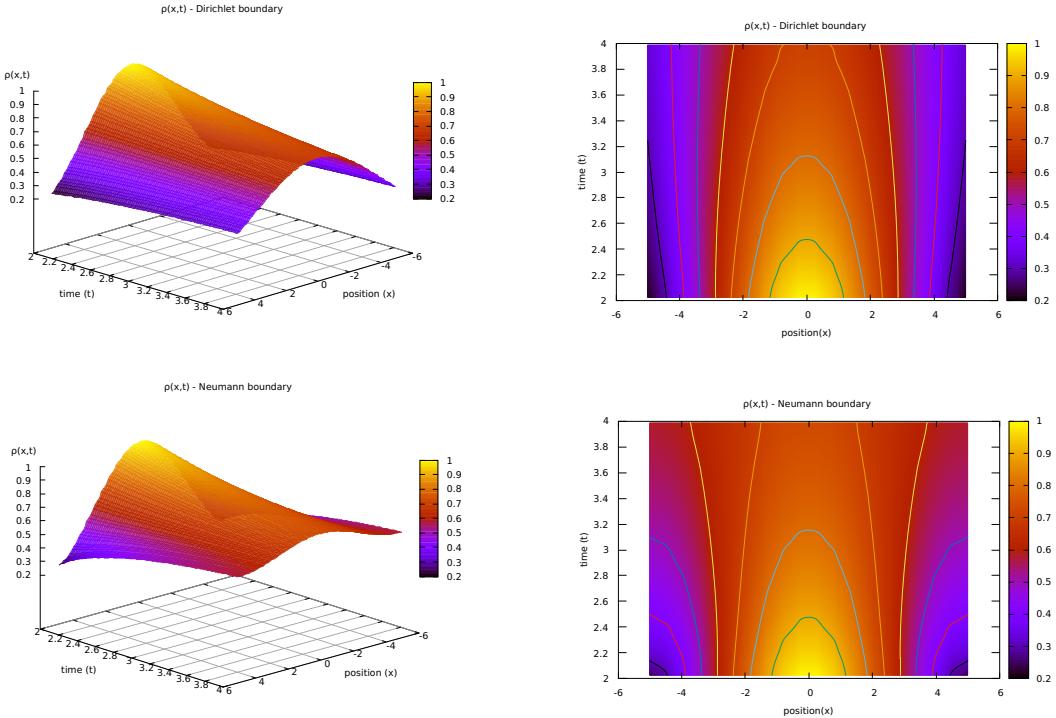
The graphical representation of the solution for both boundary conditions at $t = 4.0$ and its comparison with the analytic solution.

The results are visualized down below:

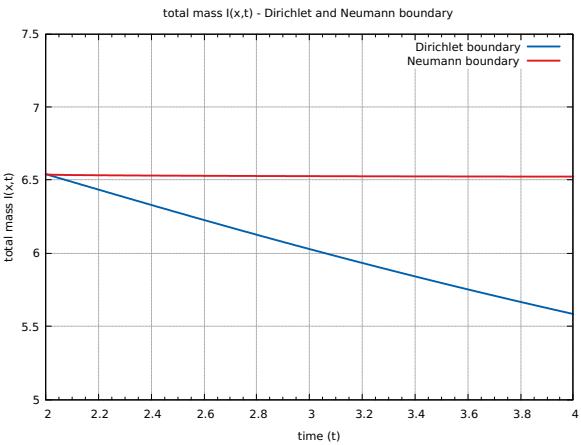


The left graphic shows the evolution of $\rho(x, t)$ and the right graphic represent the solution for $\rho(x, t)$ at $t = 4.0$. We see that the implementation by the Dirichlet boundaries are almost identical with the analytical solution, whereas the solution with Neumann boundaries differ clearly from the aforesaid.

For a better representation we have plotted the Dirichlet and the Neumann boundary approach as a 3D plot and as contour plot that show $\rho(x, t)$ over the time period $t \in [2.0, 4.0]$.



The total mass inside the computational domain as a function of time in the interval $t \in [2.0, 4.0]$ for each boundary condition. Provide an explanation for the observed trends.



We see that the total mass $I(x,t)$ inside the computational domain as a function of time in the interval $t \in [2.0, 4.0]$ for the Neumann boundary remains constant, whereas the total mass $I(x,t)$ of the Dirichlet boundary declines over time. The reason is that a Dirichlet boundary condition is one which allows for flow to occur at a boundary. A Neumann boundary condition does not allow for flow to occur at a boundary. To calculate the integral of the total mass $I(x,t)$ we use

Simpson's 1/3 rule, which is given by

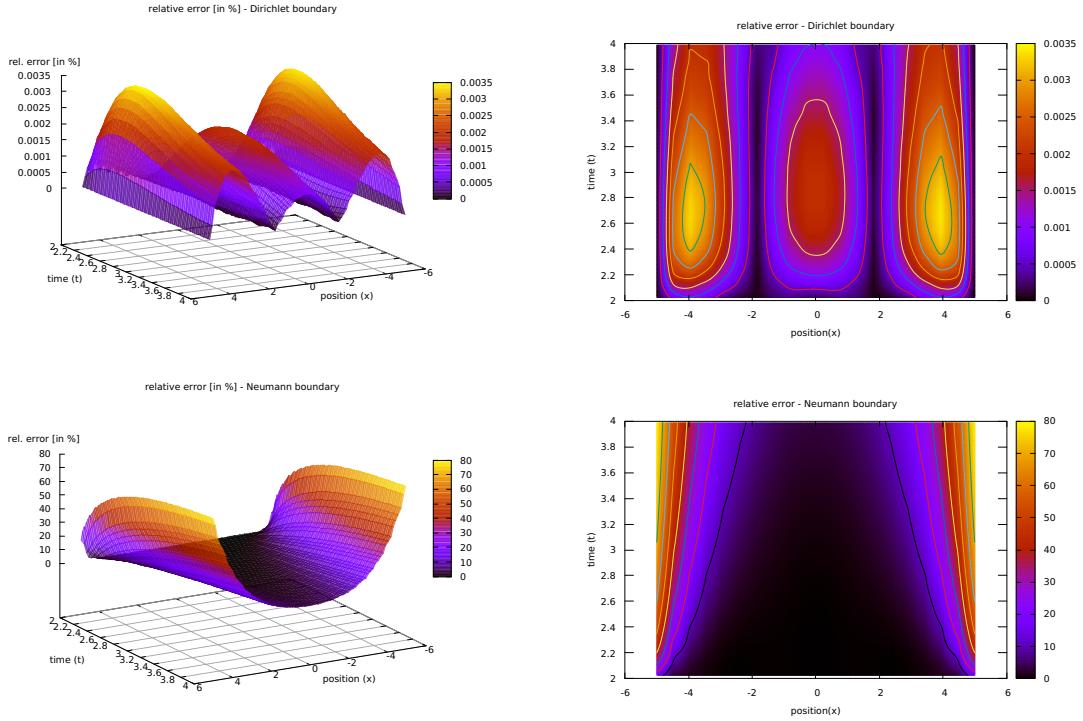
$$\int_a^b f(x)dx \approx \frac{b-a}{6} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right). \quad (12)$$

Because we have 99 grid points by construction and thus an odd number of integration points we use the Simpson's 3/8 rule, which is given by

$$\int_a^b f(x)dx \approx \frac{b-a}{8} \left(f(a) + 3f\left(\frac{2a+b}{2}\right) + 3f\left(\frac{a+2b}{2}\right) + f(b) \right), \quad (13)$$

for the last integration point to get a better approximation.

The analysis of the relative error between the numerical and exact solutions as a function of position x (also in the graphical form). Where are the minimum and maximum relative errors found (provide values)?



We see that the relative errors for the Dirichlet boundary approach at $x = -2$ and $x = 2$ and at the boundaries (obviously because of the chosen boundary conditions) are constantly almost zero over time. The largest deviation for the Dirichlet boundaries occurs at the positions $x = -4$ and $x = 4$ at approx. $t = 2.6$. For the Neumann boundary condition the relative errors appear at the boundaries as highest and increase over time.

Further remarks:

We also have implemented a small sanity-check that solve the linear system by the lapack function **gesv**. To compile the program one need to include the lapack routines. The plots where made

with GNUPLOT (Version 5.2).

Compile program: **gfortran diffusion.f90 -llapack -lblas -L~/lapack -O3 -W**

Output of the program diffusion.f90: **graphplot.txt** including the calculated densities $\rho(x, t)$, **integral.txt** including the total mass $I(x, t)$, **graphplotana.txt** including the analytical solution and **graphplotana _N.txt** including the $\rho(x, t_N)$ for $t_n = 4.0$.