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Worksheet 10
Sample Solutions

Partial Differential Equations

(H) Exercise 1: Von Neumann Stability Analysis

Consider the one-dimensional heat equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad x \in (0,1)$$

together with boundary conditions $u(t,0) = u(t,1) = 0$. We apply two different discretization schemes using explicit and implicit Euler time-stepping and the standard second-order approximation of the spatial derivative:

Explicit:

$$\frac{u_j^{(m+1)} - u_j^{(m)}}{\tau} = \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{h^2} \tag{1}$$

Implicit:

$$\frac{u_j^{(m+1)} - u_j^{(m)}}{\tau} = \frac{u_{j-1}^{(m+1)} - 2u_j^{(m+1)} + u_{j+1}^{(m+1)}}{h^2} \tag{2}$$

where h and τ denote mesh-size and time step and $u_j^{(m)} := u(m\tau, jh)$.

According to the von Neumann stability analysis, we assume the error in the solution to be of the type

$$u_j^{(m)} = (a_k)^m \sin(\pi k(jh)).$$

(a) Derive an explicit formula for the coefficient a_k in case of the explicit time-stepping, see equation 1. You may use the equality $\sin(A+B) + \sin(A-B) = 2\sin(A)\cos(B)$.

(b) Typically, the error is not given by a single frequency, but by a superposition of several frequencies k,

$$u_j^{(m)} = \sum_k c_k (a_k)^m \sin(\pi k j h).$$

Why is it enough to only consider single frequencies? What is the maximum frequency that we need to consider?

(c) The error in the solution decays if it holds $|a_k| < 1$ for all coefficients a_k. Which condition do we have to satisfy for the explicit time-stepping scheme in order to achieve this?

(d) Carry out the analysis from (c) for the implicit time-stepping scheme. Which condition arises in this case?

Solution:

(a) Inserting the definition of $u_j^{(m)}$ into the explicit time-stepping scheme yields:

$$\begin{aligned}
u_j^{(m+1)} &= a_k^{m+1} \sin(\pi k j h) \\
&\stackrel{!}{=} u_j^{(m)} + \tau \frac{u_{j-1}^{(m)} - 2u_j^{(m)} + u_{j+1}^{(m)}}{h^2} \\
&= a_k^m \sin(\pi k j h) + \\
&\quad \frac{\tau}{h^2}\left(a_k^m \sin(\pi k (j-1) h) - 2a_k^m \sin(\pi k j h) + a_k^m \sin(\pi k (j+1) h)\right) \\
&\stackrel{\substack{\sin(A+B)+\sin(A-B) \\ = 2\sin(A)\cos(B)}}{=} a_k^m \sin(\pi k j h) + \frac{\tau}{h^2}\left(a_k^m \cdot 2 \cdot \sin(\pi k j h)\cos(\pi k h) - 2a_k^m \sin(\pi k j h)\right)
\end{aligned}$$

Dividing by $a_k^m \sin(\pi k j h)$ results in an expression for a_k:

$$a_k = 1 + \frac{2\tau}{h^2}(\cos(\pi k h) - 1)$$

(b) It is enough to consider a single frequency since both the continuous and the discrete representation of the heat equation are *linear equations*. If we have two functions u and v which satisfy equation (1), then $\lambda \cdot u + \mu \cdot v$ with coefficients λ, μ also satisfy the equation.

Assume we have an equidistant discretization in space with $N+1$ points; the mesh-size is $h = 1/N$, respectively. For each point jh, consider the frequencies $\sin(\pi \cdot 0 \cdot (jh)) = 0$ and $\sin(\pi \cdot N(jh)) = \sin(\pi \cdot j) = 0$. Both functions are zero in all grid points which implies that the high frequency $\sin(\pi N x)$ cannot be sufficiently resolved on our grid. It is enough to investigate a_k for $0 < k < N$. If $k = 0$, the corresponding error frequency is already zero. If $k \geq N$, the frequency cannot be resolved on our grid.

(c) For all cases $0 < k < N$, we see that the term $\cos(\pi k h) \in (-1, 1)$ is monotonously decreasing on this interval for increasing k. We can hence check the behavior of a_k at the respective boundaries $\cos(\pi k h) \stackrel{!}{=} \pm 1$.

For $\cos(\pi k h) = 1$, we obtain $a_k = 1$, and for $\cos(\pi k h) = -1$, we have $a_k = 1 - \frac{4\tau}{h^2} < 1$. Due to the monotonous decrease of a_k, we see that $a_k < 1$ is always fulfilled on the interval $\cos(\pi k h) \in (-1, 1)$. In order to satisfy $a_k > -1$, it is required that

$$1 - \frac{4\tau}{h^2} > -1 \quad \Leftrightarrow \frac{\tau}{h^2} < \frac{1}{2}.$$

If we want to reduce our spatial resolution by a factor of two, we need to reduce our time step by a factor of four to remain stable!

(d) For the implicit time-stepping scheme, we can again compute the coefficients a_k the same way as for the explicit scheme. The coefficients are given by

$$a_k = \frac{1}{1 - \frac{2\tau}{h^2}(\cos(\pi k h) - 1)}.$$

Using the monotony of $\cos(\pi k h)$ as in the previous part of this exercise, it is enough to consider the extreme cases $\cos(\pi k h) \stackrel{!}{=} \pm 1$. We obtain

$$a_k \overset{\cos(\pi k h)\stackrel{!}{=}1}{=} 1$$

$$a_k \overset{\cos(\pi k h)\stackrel{!}{=}-1}{=} \frac{1}{1 + \frac{4\tau}{h^2}}$$

On the interval $\cos(\pi k h) \in (-1, 1)$, $|a_k| < 1$ is consequently fulfilled for *all choices of* τ *and* h. Our time-implicit algorithm is hence unconditionally stable.

(H) Exercise 2: Wave Equation

Consider the wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$$

on the interval $x \in (0, 1)$ with initial conditions

$$u(t = 0, x) = e^{-100(x-0.4)^2}, \quad \frac{\partial u(t = 0, x)}{\partial t} = 0$$

and boundary conditions

$$u(t, x = 0) = u(t, x = 1) = 0.$$

Write a python script to solve this problem using finite differences on an equidistant grid with $N + 1$ grid points. The mesh-size is denoted by $h := 1/N$ and the time step by τ.

(a) Discretize the temporal and spatial derivatives and formulate an update rule

$$u((m+1)\tau, ih) = f\left(u(m\tau, ih), u(m\tau, (i+1)h), u(m\tau, (i-1)h), u((m-1)\tau, ih)\right)$$

where $i \in \{1, ..., N-1\}$, $m \in \mathbb{N}$.

(b) How can we include the initial condition?

(c) A formula that incorporates this particular initial condition and also preserves the accuracy of the scheme is given by

$$u(\tau, ih) := u(0, ih) + \frac{\tau^2}{2h^2}(u(0, (i-1)h) - 2u(0, ih) + u(0, (i+1)h)$$

and setting $u(t = 0, ih)$ as described above. Implement both your and this approach for the initial conditions in a python script and solve the problem for $\tau \in \{0.01, 0.02\}$, $N = 90$. Plot the solution in every time step and compare the results according to your initial condition. You may consider the time interval $t \in [0, 1]$. What do you observe?

(d) Find the time step restriction from the von Neumann stability analysis.

Solution:

(a) Standard discretization using the second-order finite differences (we set $u_i^{(m)} := u(m\tau, ih)$)

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &\approx \frac{u_{i-1}^{(m)} - 2u_i^{(m)} + u_{i+1}^{(m)}}{h^2} \\ \frac{\partial^2 u}{\partial t^2} &\approx \frac{u_i^{(m+1)} - 2u_i^{(m)} + u_i^{(m-1)}}{\tau^2} \end{aligned}$$

yields:

$$u_i^{(m+1)} = \frac{\tau^2}{h^2}\left(u_{i+1}^{(m)} + u_{i-1}^{(m)}\right) + 2\left(1 - \frac{\tau^2}{h^2}\right) u_i^{(m)} - u_i^{(m-1)}$$

(b) The problem we have to face is that, in order to start the time-stepping, we need to provide at least *two values of u over time*. Therefore, we need to incorporate the gradient expression $\dfrac{\partial u(t = 0, x)}{\partial t} = 0$ into our initial condition. The simplest approach using finite differences is to approximate the gradient by

$$0 = \frac{\partial u(t = 0, x)}{\partial t} \approx \frac{u_i^{(1)} - u_i^{(0)}}{\tau}.$$

We can hence set $u_i^{(0)}$ according to the given function from above and $u_i^{(1)} = u_i^{(0)}$.

(c) See ws9_ex2.py. For $\tau = 0.02$, the solution becomes unstable and explodes. It can be shown by stability analysis that the time step and the mesh-size need to satisfy $\tau/h \leq 1$ for the present case. For $\tau = 0.01$ and $N = 90$, we have $\tau/h = 0.9 < 1$ and for $\tau = 0.02$, we obtain $\tau/h = 1.8 > 1$; the latter is beyond the stability range. The difference in the solution at $t = 1$ for the two different initial conditions is not visible from the default python plots. Still, it should be noted that the simple initial condition does not have same order of accuracy (O(τ) instead of O(τ^2) as in the second case).

(d) Next, we will find the restrictions of the time step size from the von Neumann stability

analysis. We constitute u_i^m by error $a_k^m \sin(\pi kih)$ in the numerical scheme

$$\begin{aligned} a_k^{(m+1)} sin(\pi kih) &= \frac{\tau^2}{h^2}(a_k^m \sin(\pi k(i+1)h) + a_k^m \sin(\pi k(i-1)h)) \\ &+ 2\left(1 - \frac{\tau^2}{h^2}\right) a_k^m \sin(\pi kih) - a_k^{m-1} \sin(\pi kih) \\ &= \frac{2\tau^2}{h^2} a_k^m \sin(\pi kih)\cos(\pi kh) + 2\left(1 - \frac{\tau^2}{h^2}\right) a_k^m \sin(\pi kih) \\ &- a_k^{m-1} \sin(\pi kih). \end{aligned}$$

After simplification we get a quadratic equation for a_k

$$a_k^2 - 2\left(\frac{\tau^2}{h^2}(\cos(\pi kh) - 1) + 1\right) a_k + 1 = 0.$$

The solution of this equation is

$$a_k = \left(1 - \frac{\tau^2}{h^2}(1 - \cos(\pi kh))\right) \pm \left[\left(1 - \frac{\tau^2}{h^2}(1 - \cos(\pi kh))\right)^2 - 1\right]^{\frac{1}{2}}.$$

By using the following notation $b = 1 - \frac{\tau^2}{h^2}(1 - \cos(\pi kh))$ we obtain

$$a_k = b \pm \left[b^2 - 1\right]^{\frac{1}{2}}.$$

If $|b| \leq 1$ then $a_k = b \pm \mathrm{i}\left[|1 - b^2|\right]^{\frac{1}{2}}$ and the module of the error amplitude is $|a_k| = b^2 + 1 - b^2 = 1$. So the numerical scheme is neutrally stable.

When $|b| > 1$ we have to consider two cases: $b > 1$ and $b < -1$.

In the first case we always get $a_k = b + \left[b^2 - 1\right]^{\frac{1}{2}} > 1$. And in the second case $a_k = b - \left[b^2 - 1\right]^{\frac{1}{2}} < -1$. To summarize, the numerical scheme is unstable when $|b| > 1$.

We have just to analyze $|b| \leq 1$ or $\left|1 - \frac{\tau^2}{h^2}(1 - \cos(\pi kh))\right| \leq 1$. Due to the monotony of $\cos(\pi kh)$ it is enough to consider two extreme cases $\cos(\pi kh) \stackrel{!}{=} \pm 1$.

$$b \overset{\cos(\pi kh)\stackrel{!}{=}1}{=} 1,$$

$$b \overset{\cos(\pi kh)\stackrel{!}{=}-1}{=} 1 - \frac{2\tau^2}{h^2}.$$

In the second case b is always less than one. Therefore, the restriction for the time step size we get from the inequality $1 - 2\tau^2/h^2 \geq -1$, which yields $\tau/h \leq 1$.

(I) Exercise 3: Bacteria Transport Equation

One-dimensional transport of some bacteria concentration $c(t,x)$ in some media can be described by the equation

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial x}(vc) - \lambda c, \tag{3}$$

where $D > 0$ denotes the diffusivity of the bacteria, v the flow velocity in x direction , and λ the death rate of the bacteria.

Assume that we want to solve the problem numerically for periodic boundary conditions and all parameters D, v, λ are constant.

(a) Formulate a finite difference scheme for equation (3) using first-order finite differences of the form

$$\frac{\partial f(x)}{\partial x} = \frac{f(x+h) - f(x)}{h}, \tag{4}$$

for the first-order derivative and the central difference scheme for the second-order derivatives. Use an equidistant grid with mesh size h in the x direction. State the order of the local discretization errors for both finite difference schemes.

Apply the explicit Euler scheme for the time derivative with time step size τ.

(b) From the von Neumann stability analysis, find the magnitude of the error a_k. Take the error in the solution of type $\epsilon_j^{(m)} = a_k^m e^{\imath\pi kjh}$. What condition does the error magnitude a_k have to satisfy such that the numerical scheme from the previous tasks is stable?

Solution:

(a) First, we apply the central difference discretization scheme to the second-order derivative and the first order scheme for the first order derivative

$$\frac{\partial c_j(t)}{\partial t} = D\frac{c_{j-1}(t) - 2c_j(t) + c_{j+1}(t)}{h^2} + v\frac{c_{j+1}(t) - c_j(t)}{h} - \lambda c_j(t).$$

The local discretization error of the central difference approximation is of order $O(h^2)$ whereas the error of the one-sided difference is $O(h)$.

Then, we can use the explicit Euler numerical scheme

$$\frac{c_j^{(m+1)} - c_j^{(m)}}{\tau} = D\frac{c_{j-1}^{(m)} - 2c_j^{(m)} + c_{j+1}^{(m)}}{h^2} + v\frac{c_{j+1}^{(m)} - c_j^{(m)}}{h} - \lambda c_j^{(m)}.$$

Finally, we get the numerical scheme for the bacteria concentration $c(t,x)$

$$c_j^{(m+1)} = \frac{D\tau}{h^2}\left(c_{j-1}^{(m)} - 2c_j^{(m)} + c_{j+1}^{(m)}\right) + \frac{v\tau}{h}\left(c_{j+1}^{(m)} - c_j^{(m)}\right) + (1 - \lambda\tau)c_j^{(m)}.$$

(b) According to the von Neumann stability analysis, we assume the error in the solution to be of type

$$\epsilon_j^{(m)} = a_k^m e^{i\pi kjh}$$

Inserting the definition of the error into the numerical scheme yields

$$a_k^{m+1} e^{i\pi kjh} = \frac{D\tau}{h^2} a_k^m \left(e^{i\pi k(j+1)h} - 2e^{i\pi kjh} + e^{i\pi k(j-1)h} \right) + \frac{\tau v}{h} a_k^m \left(e^{i\pi k(j+1)h} - e^{i\pi kjh} \right) + (1 - \tau\lambda) a_k^m e^{i\pi kjh}.$$

Dividing this expression by $a_k^m \exp(i\pi kjh)$ and using the equality

$$(\exp(i\pi kh) + \exp(-i\pi kh))/2 = \cos(\pi kh)$$

results in an expression for a_k

$$a_k = 1 - \lambda\tau + \frac{2D\tau}{h^2}(\cos(\pi kh) - 1) + \frac{\tau v}{h} \left(e^{i\pi kh} - 1 \right).$$

After simplifications we get:

$$a_k = 1 - \lambda\tau + \left(\frac{2D\tau}{h^2} + \frac{\tau v}{h} \right) (\cos(\pi kh) - 1) + i \frac{\tau v}{h} \sin(\pi kh).$$

To obtain a stable numerical scheme for our problem, the error magnitude should be $|a_k| \leq 1$, so that numerical errors do not grow with each time step.

(H*) Exercise 4: Free Charges in Semiconductors

There are semiconductors that do not conduct electric current unless they are exposed to light. Free electrons appear in this material due to the photo-effect. They can again get trapped and localized.

(a) A thin layer of semiconductor has momentarily been exposed to light. This created a homogeneous density n_0 of free electrons. Write down the ODE for the free electrons density $n(t)$ and solve it if free electrons get trapped again at a rate $wn(t)$ (number of free electrons trapped in a unit volume per unit time interval). What is $n(t \to \infty)$?

(b) To improve the model, potential holes are introduced. In our model, potential holes will only keep one electron at the same time. If M is the number of potential holes, $m(t) = n_0 - n(t)$ is the number of localized electrons, then $\alpha(1 - m(t)/M)n(t)$ is number of trapped electrons in the potential holes per unit time interval. And the number of electrons that get free again per unit time interval is $\beta m(t)$. The resulting ODE is

$$\frac{\mathrm{d}n(t)}{\mathrm{d}t} = \beta(n_0 - n(t)) - \alpha \left(1 - \frac{n_0 - n(t)}{M} \right) n(t). \tag{5}$$

For $n_0 = 1, M = 1, \alpha = 2, \beta = 1$ find a physical ($n \geq 0$) stationary solution for the free electron concentration n_s of this equation.

(c) Determine whether the physical ($n \geq 0$) stationary solution from (b) is stable.

(d) If the semiconductor layer is thick, the generated density of free electrons n is no longer homogeneous. More electrons are freed near the surface and less inside the layer. The simplest model for the evolution of $n(x,t)$ considers diffusion along the layer depth x and is described by the following equation

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} - \gamma n, \tag{6}$$

where the coefficients D and γ are positive.

Provide a numerical scheme for this PDE. For the time discretization use the explicit Euler scheme and for the spatial discretization a central difference second-order scheme. For an example of a discretization grid see Figure 1.

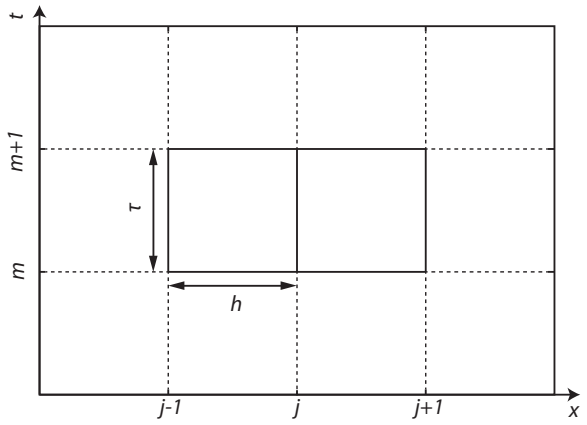

Figure 1: Discretization grid example.

(e) Find the restriction for the time step size of the numerical scheme by using the von Neumann stability analysis.

Solution:

(a) The differential equation describing the model is 0.5

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -wn$$

The solution of this equation

$$\begin{aligned} \frac{\mathrm{d}n}{n} &= -w\,\mathrm{d}t, \\ \ln(n) &= -const \cdot wt, \\ n(t) &= n_0 e^{-wt}. \end{aligned}$$

The solution asymptotically approaches $n(t \to \infty) = 0$.

(b) With given parameters $n_0 = 1, M = 1, \alpha = 2, \beta = 1$ we obtain the following ODE

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -2n^2 - n + 1.$$

The stationary solution n_s corresponds to the critical points and defined by the quadratic equation

$$-2n^2 - n + 1 = 0.$$

The solution of the quadratic equation gives two possible n_s:

$$n_s = \frac{-1 \pm 3}{4}.$$

But only one of the solutions is physical (the free electron density must be positive) $n_s = 1/2$.

(c) Now, the ODE has the form

$$\frac{\mathrm{d}n}{\mathrm{d}t} = -2n^2 - n + 1.$$

The physical stationary solution of this equation is $n_s = 1/2$.

To possible ways to obtain the stability of a critical point exist.

One can either consider the area around the point by checking the behavior of a slightly disturbed electron density. Therefor we take a small $\epsilon > 0$ and consider the deviation from the critical point:

$$\begin{aligned}
n = n_s + \epsilon, \quad \frac{\mathrm{d}n}{\mathrm{d}t} &= -2(n_s + \epsilon)^2 - n_s - \epsilon + 1 \\
&= -2n_s^2 - n_s + 1 - 4n_s\epsilon - 2\epsilon^2 - \epsilon \\
&= -(4n_s + 1)\epsilon - 2\epsilon^2 = -3\epsilon - 2\epsilon^2 < 0, \\
n = n_s - \epsilon, \quad \frac{\mathrm{d}n}{\mathrm{d}t} &= -2(n_s - \epsilon)^2 + n_s - \epsilon + 1 \\
&= -2n_s^2 - n_s + 1 + 4n_s\epsilon - 2\epsilon^2 + \epsilon \\
&= (4n_s + 1)\epsilon - 2\epsilon^2 = 3\epsilon - 2\epsilon^2 > 0, \quad \text{for sufficiently small } \epsilon
\end{aligned}$$

We thus see, that a positive deviation from the critical point yields a negative time derivative for the electron density. Latter will thus decrease until it has reached the critical density. Likewise a negative deviation yields an increase in the electron density.

The other possibility is to check the equation directly:

$$\begin{aligned}
\frac{\mathrm{d}n}{\mathrm{d}t} &= -2n^2 - n + 1 \\
\frac{\mathrm{d}}{\mathrm{d}n}\frac{\mathrm{d}n}{\mathrm{d}t} &= -4n - 1
\end{aligned}$$

Evaluating the upper equation on the critical point $n^* = \frac{1}{2}$ yields $\frac{\mathrm{d}}{\mathrm{d}n}\frac{\mathrm{d}n}{\mathrm{d}t} = -3 < 0$. We can thus conclude, that the critical point is stable.

(d) First, we apply a central difference discretization scheme to the second-order derivative

$$\frac{\partial n_j(t)}{\partial t} = D\frac{n_{j-1}(t) - 2n_j(t) + n_{j+1}(t)}{h^2} - \gamma n_j(t).$$

Then we can use the explicit Euler scheme

$$\frac{n_j^{(m+1)} - n_j^{(m)}}{\tau} = D\frac{n_{j-1}^{(m)} - 2n_j^{(m)} + n_{j+1}^{(m)}}{h^2} - \gamma n_j^{(m)}$$

Finally, we obtain the numerical scheme for free electrons density $n(t, x)$

$$n_j^{(m+1)} = \frac{D\tau}{h^2}\left(n_{j-1}^{(m)} - 2n_j^{(m)} + n_{j+1}^{(m)}\right) + (1 - \gamma\tau)n_j^{(m)}$$

(e) According to the von Neumann stability analysis, we assume the error in the solution to be of type

$$\epsilon_j^{(m)} = a_k^m e^{\imath\pi kjh}$$

Inserting the definition of the error into the numerical scheme yields

$$a_k^{m+1}e^{\imath\pi kjh} = \frac{D\tau}{h^2}a_k^m\left(e^{\imath\pi k(j+1)h} - 2e^{\imath\pi kjh} + e^{\imath\pi k(j-1)h}\right) + (1 - \tau\gamma)a_k^m e^{\imath\pi kjh}.$$

Dividing this expression by $a_k^m \exp(\imath\pi kjh)$ and using the equality

$$(\exp(i\pi kh) + \exp(i\pi kh))/2 = \cos(\pi kh)$$

results in an expression for a_k

$$a_k = 1 - \gamma\tau + \frac{2D\tau}{h^2}(\cos(\pi kh) - 1).$$

Due to the monotony of $\cos(\pi kh)$, it is enough to consider the extreme cases $\cos(\pi kh) \stackrel{!}{=} \pm 1$. For $\cos(\pi kh) \stackrel{!}{=} 1$ we get

$$a_k = 1 - \tau\gamma,$$

and for $\cos(\pi kh) \stackrel{!}{=} -1$ we obtain

$$a_k = 1 - \tau\gamma - \frac{4D\tau}{h^2}.$$

In the both cases we get $a_k < 1$ and in the second case we get a smaller a_k. Therefore, we have to consider only the inequality

$$1 - \tau\gamma - \frac{4D\tau}{h^2} > -1,$$

from which follows the restriction for the time step size:

$$\tau < \frac{1}{2D/h^2 + \gamma/2}.$$