Partial Differential Equations (PDEs)

Primary Reference: "*Numerical Methods for Physics*" by A. Garcia, Chapters 6-9

Much of computational physics is devoted to solving PDEs of some form or another. The numerical solution of PDEs is a vast and complex area of study. We can only hope to scratch the surface here.

Classification of PDEs

There are 2 classes of problems:

Initial value problems such as the *wave equation* is a hyperbolic equation

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2}$$

Or the diffusion equation which is a parabolic equation

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\kappa \frac{\partial u(x,t)}{\partial x}\right)$$

The task here is given $u(x,0)$, find $u(x,t)$

The third type are elliptic equations such as Poisson's equation

where $\Phi(x,y)$ or a normal gradient is given at the boundary

to be covered later

$$\frac{\partial^2 \Phi(x,y)}{\partial x^2} + \frac{\partial^2 \Phi(x,y)}{\partial y^2} = -\frac{1}{\varepsilon_0}\rho(x,y)$$

Classification of PDEs

The following 2nd order PDE

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu = g$$

Where *a*-*g* can be constants or given functions (non-linear).

There are 3 basic types of PDES:

(a) parabolic: $b^2 - 4ac = 0$, *e.g.*, $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ *(diffusion)*

(b) hyperbolic: $b^2 - 4ac > 0$, *e.g.*, $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$ *(wave)*

(c) elliptic $b^2 - 4ac < 0$, *e.g.*, $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}$ *(Laplace)*

Classification of PDEs (cont.)

- Hyperbolic PDEs described time dependent, conservative physical processes that are *not* evolving towards a steady state
  - Conservative means energy, mass, etc
  - Can produce non-smooth solutions (e.g. shocks)
  - Are time reversible, in principal
- Parabolic PDEs describe time dependent, dissipative physical processes that *are* evolving towards a steady state
  - Dissipative means that energy, mass etc are not constant
  - Typically have exponentially decaying solutions
  - Typically yield smooth solutions
  - Are time irrreversible
- Elliptic PDEs describe physical systems that have reached steady state, or equilibrium and are time-independent.

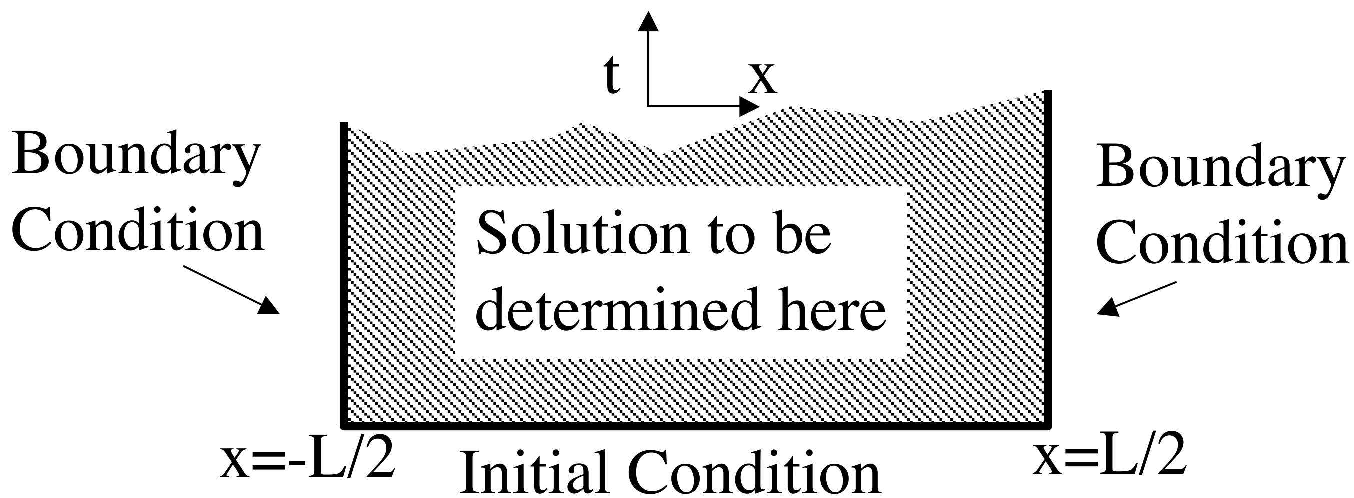
Initial Value Problems

Hyperbolic and Parabolic equations are both treated as initial value problems.

For the diffusion equation for temperature, T(x,t)

$$\frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(\kappa \frac{\partial T(x,t)}{\partial x}\right)$$

One would be given the initial *T(x,0)* and some boundary condition since the solution is likely constrained to some region of space



Boundary Conditions

Consider the Diffusion equation as applied to the Heat equation, *T(x,t)* is then the temperature

Dirichlet Boundary Conditions

$$T(-L/2,t) = T_a \qquad T(L/2,t) = T_b$$

where the temperature T has been specified at the boundary

Neumann Boundary (Flux) Conditions

$$-\kappa \left.\frac{dT}{dx}\right|_{x=-L/2} = F_a \qquad -\kappa \left.\frac{dT}{dx}\right|_{x=L/2} = F_b$$

which specifies the heat flux at the boundaries

Another Boundary condition we could use is *Periodic boundary conditions*

$$T(-L/2,t) = T(L/2,t) \qquad \left.\frac{dT}{dx}\right|_{x=-L/2} = \left.\frac{dT}{dx}\right|_{x=L/2}$$

Discretization

Numerical solutions of PDEs produce a solution on a grid, both space and time are discretized

Discretization *N* evenly space points in space in 1D on a line length L as

$$x_i = -\frac{L}{2} + \frac{i-1}{N-1}L$$

or

$$x_i = -\frac{L}{2} + (i-1)h$$

where *h* is the grid spacing $h = \frac{L}{N-1}$

Time is also discretized as $t_n = (n-1)\tau$

The solution is evolved in time a what is called a *marching method* where the solution is computed one step into the future

1D Diffusion Equation

Method of Images

Start with the equation, where κ is a constant

$$\frac{\partial T(x,t)}{\partial t} = \kappa \frac{\partial^2 T(x,t)}{\partial x^2}$$

where κ is a constant. A solution can be verified to be a Gaussian

$$T_G(x,t) = \frac{1}{\sqrt{4\pi\kappa t}}\, e^{-\left[\frac{(x-x_0)^2}{4\kappa t}\right]}$$

Note that

$$\int_{-\infty}^{\infty} T_G(x,t)\,dx = 1$$

and

$$\lim_{t\to\infty} T_G(x,t) = \delta(x - x_0)$$

Method of Images

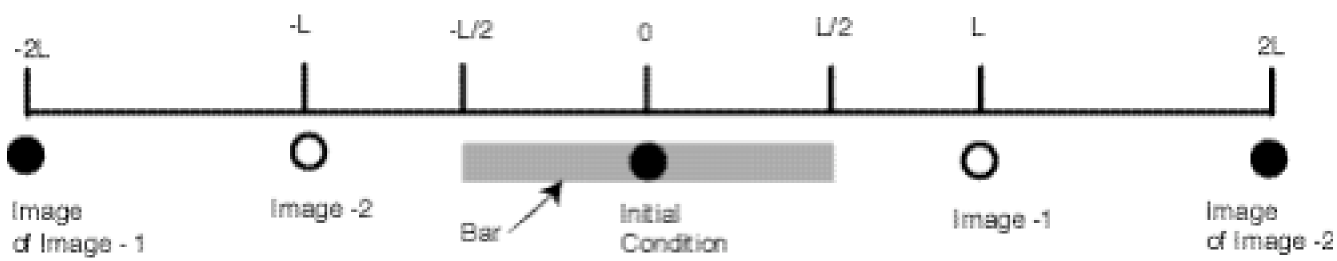
The method of images can be used to solve the diffusion equation with the boundary condition $T(x,t=0)=\delta(x)$ with the Dirichlet boundary condition

$$T(-L/2,t) = T(L/2,t) = 0$$

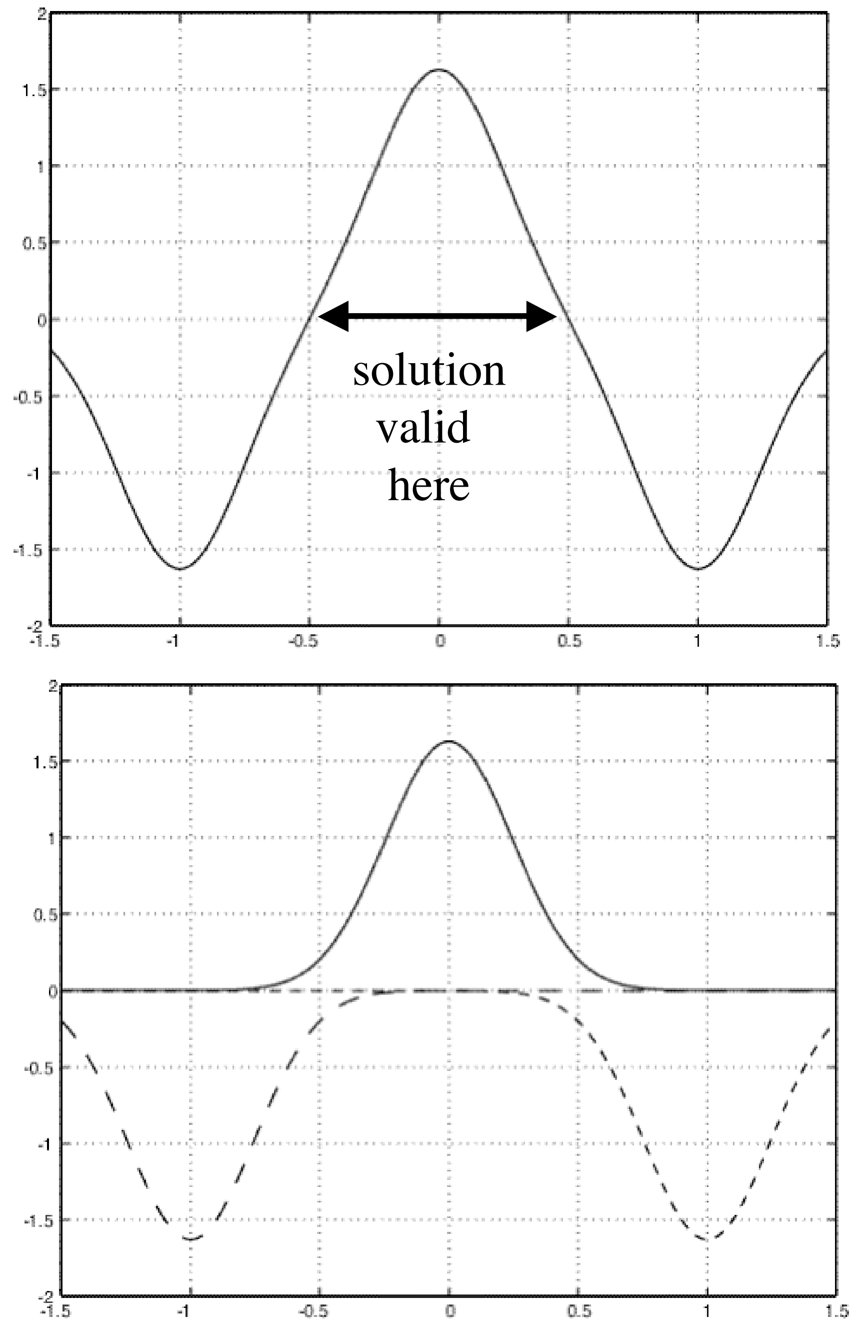
So we have to find $T(x,t)$.

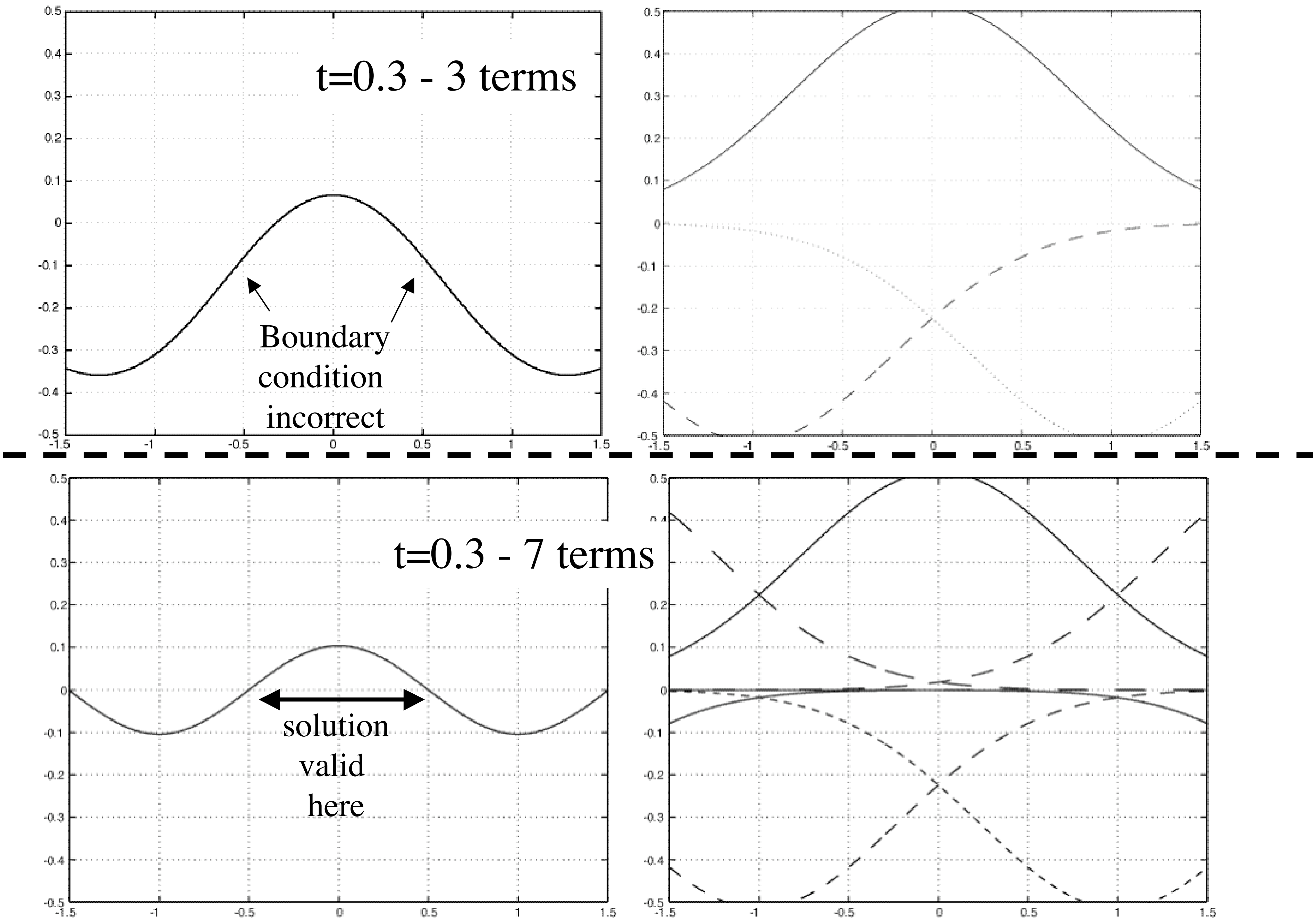
The method of images can be used to construct the solution

$$T(x,t) = \sum_{n=-\infty}^{\infty} (-1)^n T_G(x+nL,t)$$



t=0.03 - 3 terms





t=0.3 - 3 terms
Boundary
condition
incorrect
t=0.3 - 7 terms
solution
valid
here

Forward in time centered in space method (FTCS)

The simplest method to numerically solve an initial value problem is with the *Forward in Time Centered in Space* (FTCS) method

Rewrite the diffusion equation in finite difference form as

$$\frac{T_i^{n+1} - T_i^n}{\tau} = \kappa \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{h^2}$$

where $T_i^n \equiv T(x_i, t_n) \equiv T(-L/2 + (i-1)h, (n-1)\tau)$

which can be rewritten as

$$T_i^{n+1} = T_i^n + \frac{\tau\kappa}{h^2}(T_{i+1}^n - 2T_i^n + T_{i-1}^n)$$

The FTCS method is an *explicit* method and is related to the Euler method for ODEs.

It can be shown to be stable when $t < \frac{h^2}{2\kappa}$

Stability analysis - Perturbation

For the equation

$$\frac{T_i^{n+1} - T_i^n}{\tau} = \kappa \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{h^2}$$

Assume that we have a solution T_i^n and introduce a disturbance ε_i^n and see what happens to it by calculating ε_i^{n+1}

$$\frac{T_i^{n+1} + \varepsilon_i^{n+1} - T_i^n - \varepsilon_i^n}{\tau} = \kappa \frac{T_{i+1}^n - 2(T_i^n + \varepsilon_i^n) + T_{i-1}^n}{h^2}$$

Subtracting these 2 equations we get

$$\frac{\varepsilon_i^{n+1}{}_i^n - \varepsilon_i^n}{\tau} = \kappa \frac{-2\varepsilon_i^n}{h^2}$$

Stability analysis - Perturbation -2

Or we get

$$\varepsilon_i^{n+1} = \varepsilon_i^n - 2\tau\kappa \frac{\varepsilon_i^n}{h^2}$$

Or

$$\frac{\varepsilon_i^{n+1}}{\varepsilon_i^n} = 1 - \frac{2\tau\kappa}{h^2} = 1 - 2d$$

Where $d = \dfrac{\tau\kappa}{h^2}$ For the disturbance to die off we want $\left|\dfrac{\varepsilon_i^{n+1}}{\varepsilon_i^n}\right| \le 1$

$$\Rightarrow |1 - 2d| \le 1$$

$$\Rightarrow 1 - 2d \le 1 \text{ and } 1 - 2d \ge -1$$

$$\Rightarrow 1 - 2d \ge -1$$

$$\Rightarrow d \le 1$$

$$\Rightarrow \frac{\tau\kappa}{h^2} \le 1 \Rightarrow \tau \le \frac{h^2}{\kappa}$$

Stability analysis 2 - Perturbation

A <u>more restrictive</u> case is where we have a perturbation on every other grid point, so that

$$T_i^n \to T_i^n + \varepsilon^n \qquad T_{i+1}^n \to T_{i+1}^n - \varepsilon^n \qquad T_{i-1}^n \to T_{i-1}^n - \varepsilon^n$$

$$\frac{T_i^{n+1} + \varepsilon_i^{n+1} - T_i^n - \varepsilon^n}{\tau} = \kappa \frac{T_{i+1}^n - \varepsilon^n - 2T_i^n + 2 - \varepsilon^n + T_{i-1}^n - \varepsilon^n}{h^2}$$

$$\Rightarrow |1 - 4d| \leq 1$$

$$\Rightarrow 1 - 4d \geq -1$$

$$\Rightarrow d \leq \frac{1}{2}$$

$$\Rightarrow \tau \leq \frac{h^2}{2\kappa}$$

Stability Analysis - Von Neumann

This is a commonly used procedure where we look at the effect of the numerical method on fourier components, if we define the solution in the form

$$T_j^n = T^n e^{ikhj}$$

$$T_j^{n+1} = T^{n+1} e^{ikhj} \qquad\qquad T_{j\pm1}^{n+1} = T^{n+1} e^{ikh(j\pm1)}$$

Placing this into the diffusion equation

$$T^{n+1} e^{ikhj} = T^n e^{ikhj} + dT^n e^{ikhj} (e^{-ikh} - 2 + e^{ikh})$$

$$A = \frac{T^{n+1}}{T^n} = 1 + 2d(\cos kh - 1)$$

Von Neumann - continued

For the method to be stable, we would require that $|A \leq 1|$ for all k. Removing the absolute value sign gives us 2 cases:

$$1 + 2d(\cos kh - 1) \leq 1$$
$$\Rightarrow 2d(\cos kh - 1) \leq 0$$

Which is always true, and

$$1 + 2d(\cos kh - 1) \geq -1$$
$$\Rightarrow 2d(\cos kh - 1) \geq -2$$

Since this must be true for all k, so we pick the smallest value of cos(kh), which is -1

$$2d(-2) \geq -2$$
$$\Rightarrow d \leq \frac{1}{2} \; or \; \tau \leq \frac{h^2}{2\kappa}$$