



*NucE 497: Reactor Fuel Performance*

**Lecture 9: 1D transient solution of  
heat equation using  
Matlab**

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Some material taken from Matlab documentation



# Today we will discuss solving for the temperature profile in the fuel using 1D transient FEM

- Module 1: Fuel basics
- Module 2: Heat transport
  - Intro to heat transport and the heat equation
  - Analytical solution of the heat equation
  - Numerical solution of the heat equation
  - **1D solution of the heat equation using Matlab**
  - 2D solution of the heat equation using Matlab
  - Coolant temperature change, power generation, and melting
- Module 3: Mechanical behavior
- Module 4: Materials issues in the fuel
- Module 5: Materials issues in the cladding
- Module 6: Accidents, used fuel, and fuel cycle



## Let's review some from last time:

- What is one strength and one weakness of the finite element method?
  - a. Can model any geometry but very complicated
  - b. Simple to implement, but limited on boundary conditions
  - c. Can model any geometry but can't hand heterogeneous properties well
  - d. Can model any boundary condition, but it required periodic boundary conditions
- What temperature solution assumes axisymmetry and that the pellets act as a single body?
  - a. 1D transient
  - b. 1.5D transient
  - c. 2D transient, smeared pellets
  - d. 2D transient, discrete pellets



## Quiz question: Which is not actually true about LWR nuclear fuel, but is assumed to make the analytical model possible?

- a) The fuel system has a cylindrical geometry
- b) The thermal conductivity of UO<sub>2</sub> is constant with temperature
- c) Heat is generated throughout the fuel pellet
- d) The fuel is solid throughout the fuel pellet during normal operation

Attempts: 33 out of 33

+0.42

Discrimination Index ⓘ

Which is not actually true about LWR nuclear fuel, but is assumed to make the analytical model possible?

The fuel system has cylindrical symmetry		0 %	
The thermal conductivity of UO <sub>2</sub> is constant with temperature	29 respondents	88 %	✓
Heat is generated throughout the fuel pellet		0 %	
The fuel is solid throughout the fuel pellet during normal operation	4 respondents	12 %	





## Quiz question: Numerical solutions for the temperature profile throughout the fuel have both strengths and weaknesses compared to analytical solutions. Which is a correct set of a strength and a weakness?

a) Strength: Accounts for human error; Weakness: More boring

Attempts: 33 out of 33

+0.24

Discrimination Index ?

Numerical solutions for the temperature profile throughout the fuel have both strengths and weaknesses compared to analytical solutions. Which is a correct set of a strength and a weakness?

Strength: Accounts for the human error Weakness: More boring		0 %	
Strength: Accounts for temperature dependence of the thermal conductivity Weakness: Does not correctly represent geometry	2 respondents	6 %	
Strength: Accounts for cylindrical symmetry Weakness: Higher computational complexity	1 respondents	3 %	
Strength: Accounts for temperature dependence of the thermal conductivity Weakness: Higher computational complexity	30 respondents	91 %	✓





**Quiz question: Early fuel performance codes used one dimensional predictions in space of the temperature profile in a fuel rod, to simplify the calculation. The dimension used in these simulations was the one that experienced the most temperature change. This dimension was the**

- a) Radial position
- b) Axial position
- c) Location with the fuel assembly

Attempts: 33 out of 33

**+0.42**

Discrimination Index ?

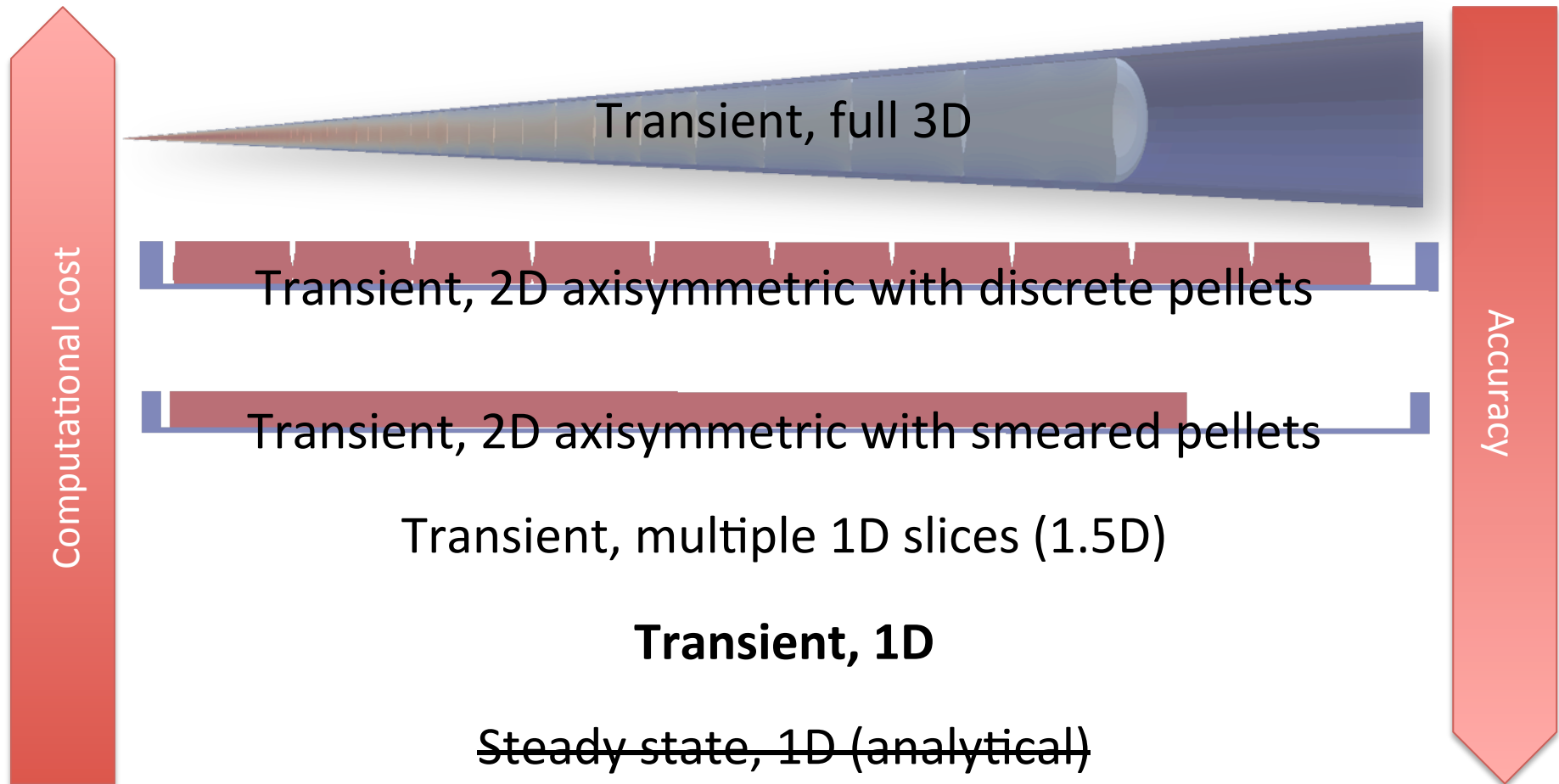
Early fuel performance codes used one dimensional predictions in space of the temperature profile in a fuel rod, to simplify the calculation. The dimension used in these simulations was the one that experienced the most temperature change. This dimension was the

Radial position	29 respondents	88 %	<div></div> ✓
Axial position	3 respondents	9 %	<div></div>
Location within the fuel assembly		0 %	<div></div>
Location within the core	1 respondents	3 %	<div></div>





# We talked about numerical methods, now we will use one for 1D transient solutions





## Remember our two assumptions

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$

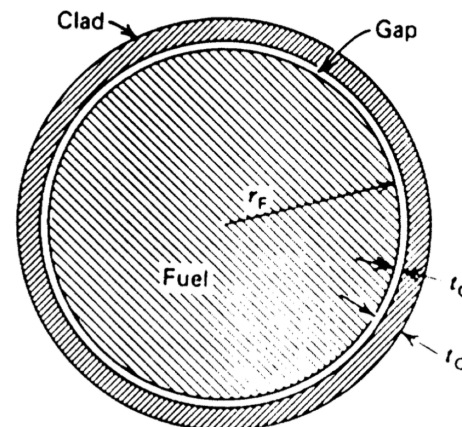
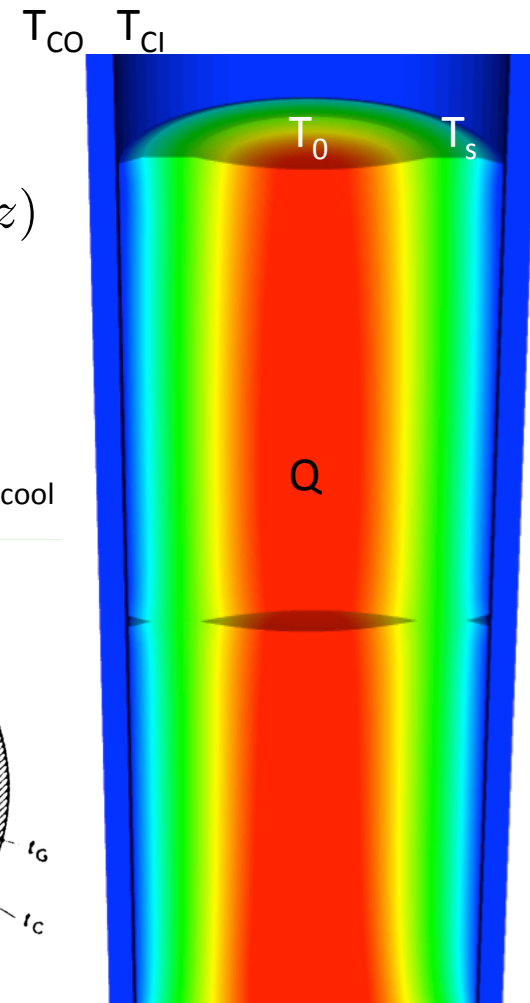
- *Assumption 1: The behavior is axisymmetric*

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left( k(T) \frac{\partial T}{\partial z} \right) + Q(r, z)$$

- *Assumption 2:  $T$  is constant in  $z$*

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k(T) \frac{\partial T}{\partial r} \right) + Q(r)$$

- **We will solve this using FEM and implicit time integration in Matlab**



Coolant





**In Matlab, you save files of commands, and when you run the file, it runs the commands**



## Matlab easily deals with vectors and matrices

- You can easily create vectors or matrices
  - $A = [1 \ 2 \ 3 \ 4];$
  - $B = [1 \ 3 \ 4 \ 5; 1 \ 3 \ 5 \ 3];$
  - $C = [8 \ 26 \ 24 \ 32];$
- Operations with a . first, like .\* or ./ operate on corresponding values in the vectors or matrices
  - $C./A = [2 \ 2 \ 2 \ 2]$



## Your saved file can define multiple functions

Function RunStuff

%This function just runs another function

vec1 = [1, 4];

vec2 = [4, 7];

[a, b] = test(vec1, vec2);

end

Function [a, b] = test(c, d)

a = c + d;

b = c.\*d;

end



# If you need to use the same quantity in multiple functions, you can make it global

- Normally, a variable only exists in the function it was created in.

```
Function RunStuff
    vec1 = [1, 4];
    vec2 = [4, 7];
    [a, b] = test(vec1, vec2);
    mult = 5;
end
```

```
THIS DOESN'T WORK!
Function [a, b] = test(c, d)
    a = mult*(c + d);
    b = c.*d;
end
```

- However, you can declare a variable global in each function and now it can be accessed

```
Function RunStuff
    global mult;
    vec1 = [1, 4];
    vec2 = [4, 7];
    [a, b] = test(vec1, vec2);
    mult = 5;
end
```

```
THIS WORKS
Function [a, b] = test(c, d)
    global mult;
    a = mult*(c + d);
    b = c.*d;
end
```



## Matlab has lots of documentation

- If you want to do something but you don't know the command, google it
- If you know the command, you can use the help command
  - In matlab > help plot



## Matlab has great capability for plotting.

- For bar plots, use the “bar” command (type help bar to learn about it)
- For line plots, use the “plot” command.
  - You pass the command two vectors of the same length, and it uses the first one for the x axis of points and the second one for the y axis
  - For example `plot([1:5], sqrt(1:5))`
- If you pass in a matrix, you can plot a surface using the “surf” command



## Matlab's 1D PDE solver is called pdepe

- pdepe solve a 1D PDE in time and in one spatial direction using a transient implicit solution in time and the finite element method in space

$$c \left( x, t, u, \frac{\partial u}{\partial x} \right) \frac{\partial u}{\partial t} = x^{-m} \frac{\partial}{\partial x} \left( x^m f \left( x, t, u, \frac{\partial u}{\partial x} \right) \right) + s \left( x, t, u, \frac{\partial u}{\partial x} \right)$$

- u is the variable we are solving for, it is a function of x and t
- x is the space variable,  $a \leq x \leq b$
- t is the time variable,  $t_0 \leq t \leq t_f$
- $m = 0, 1, \text{ or } 2$
- How can we make this equation match our heat equation?

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k(T) \frac{\partial T}{\partial r} \right) + Q(r)$$

- What is u? What is x? What is t? What is m? What is c? What is f? What is s?



## We make the solution fit the heat equation by correctly setting the parameters

$$c \left( x, t, u, \frac{\partial u}{\partial x} \right) \frac{\partial u}{\partial t} = x^{-m} \frac{\partial}{\partial x} \left( x^m f \left( x, t, u, \frac{\partial u}{\partial x} \right) \right) + s \left( x, t, u, \frac{\partial u}{\partial x} \right)$$
$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r k(T) \frac{\partial T}{\partial r} \right) + Q(r)$$

- $x = r, t = t, u = T, dU/dx = dT/dr$
- $m = 1$
- $c(x, t, u, du/dx) = \rho c_p$
- $f(x, t, u, du/dx) = k(T) dT/dr$
- $s(x, t, u, du/dx) = Q(r)$





## In order to use PDEPE, we have to provide six inputs

**`sol = pdepe(m, @PDEfunction, @ICfunction, @BCfunction, r, t);`**

- The input `m` sets the coordinate system (`m = 0` for Cartesian, `m = 1` for cylindrical, and `m = 2` for spherical)
- We need to create three functions
  - `[c, f, s] = PDEfunction(x, t, u, dudx)` – This function defines the three constants in the PDE
  - `u = ICfunction(x)` – This function defines the initial condition of `u`
  - `[pl, ql, pr, qr] = BCfunction(xl, ul, xr, ur, t)` – This function defines boundary conditions on the left and right side of the domain
- We create the mesh using the command `r = linspace(a, b, N)`
  - This creates `r` as a vector that goes from `a` to `b` with `N` points
- We create the time domain `t = linspace(t0, ts, M)`
  - This creates `t` as a vector that goes from `t0` to `ts` with `M` time steps



## Here is more detail about the function that creates the three terms of the PDE

**[c, f, s] = PDEfunction(x, t, u, dudx)**

$$c \left( x, t, u, \frac{\partial u}{\partial x} \right) \frac{\partial u}{\partial t} = x^{-m} \frac{\partial}{\partial x} \left( x^m f \left( x, t, u, \frac{\partial u}{\partial x} \right) \right) + s \left( x, t, u, \frac{\partial u}{\partial x} \right)$$

- Four inputs are passed in by the solver
  - x – the current location in space (r in our case)
  - t – the current time
  - u – the current value of the variable (T in our case)
  - dudx – the current value of the derivative of the variable (dT/dr in our case)
- You then define c, f, and s as functions of these variables

```
function [c,f,s] = PDEfunction(x,t,u,DuDx)
    global density cp Q k

    c = density*cp;
    f = k*DuDx;
    s = Q;

end
```



## Here is more detail about the function that creates the initial condition

$$u = \text{ICfunction}(x)$$

- One input is passed in by the solver
  - $x$  – the current location in space ( $r$  in our case)
- You then define the value of the variable throughout the mesh at  $t = 0$

```
function u0 = ICfunction(x)
    global Ts;
    %Initial temperature
    T0 = Ts; %K

    %Assign values
    u0 = T0*ones(size(x));
end
```



## Here is more detail about the function that creates the boundary condition

$$[pl, ql, pr, qr] = \text{BCfunction}(xl, ul, xr, ur, t)$$

- Five inputs are passed in by the solver
  - $xl$  – the coordinate location on the left side ( $r = 0$  in our case)
  - $ul$  – the value of  $u$  on the left side ( $T(r=0)$  in our case)
  - $xr$  – the coordinate location on the right side ( $r = R_f$  in our case)
  - $ur$  – the value of  $u$  on the right side ( $T(r=R_f)$  in our case)
- You define the boundary conditions on the left and right side in this form:

$$p(x, t, u) + q(x, t) f\left(x, t, u, \frac{\partial u}{\partial x}\right) = 0$$

- $pl$  and  $ql$  set  $p$  and  $q$  on the left. These are ignored for cylindrical and spherical coordinates
- $pr$  and  $qr$  set  $p$  and  $q$  on the right.
- What are  $p$  and  $q$  for  $T_r = T_s$ ?
  - $pr = ur - T_s$

```
function = BCfunction(xl,ul,xr,ur,t)
global Ts;

pl = 0; %This gets ignored
ql = 0; %This gets ignored
pr = ur - Ts;
qr = 0;

end
```

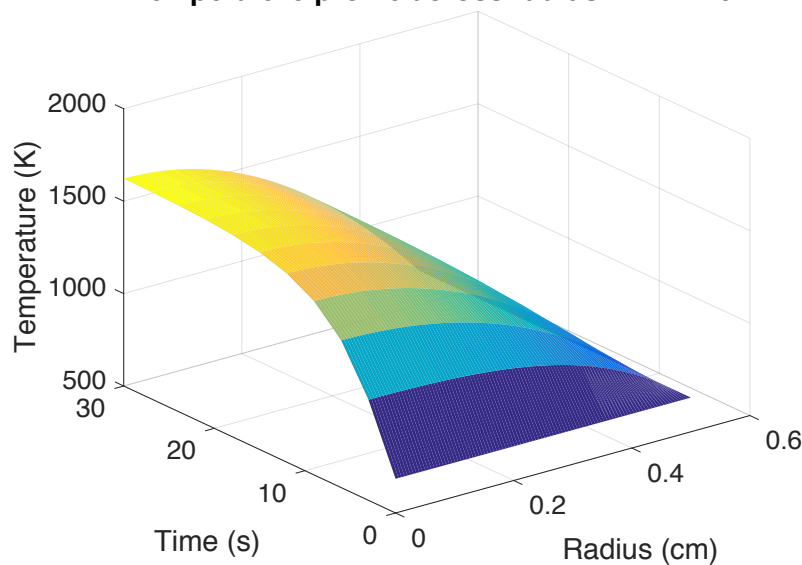


## The solution comes out as a 3D array of data

`T = pdepe(1,@PDEfunction,@ICfunction,@BCfunction,r,t);`

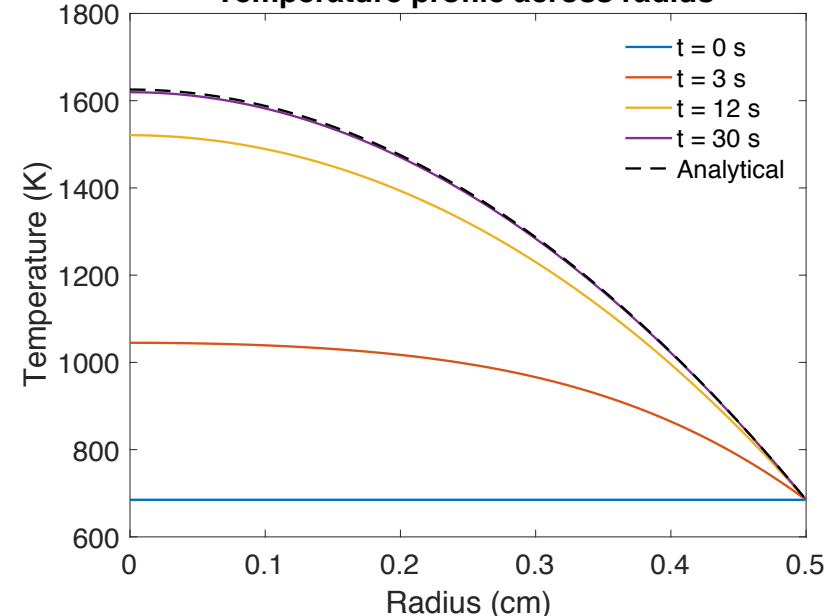
- The 1<sup>st</sup> dimension is the spatial coordinate, the 2<sup>nd</sup> is the time coordinate, and the third is for additional variables you may be solving for.
- So, if we solve just for T on a mesh with N nodes and M times steps, T is a  $N \times M$  matrix
- You could plot it in various ways

Temperature profile across radius with time



`surf(r, t, T, 'edgecolor','none')`

Temperature profile across radius



`plot(r, T([1,2,5,10],:),'linewidth',1.5)`



## Now, let's look at the code

The image shows the MATLAB R2016a - academic use interface. The main window displays a script named `rod_temp_profile_simple.m` with the following code:

```
1 function rod_temp_profile_simple
2     clear
3     close all
4
5     global density cp Q Ts k
6
7     %Material Properties
8     k = 0.03; %W/(cm K), thermal conductivity of UO2 at higher temperature
9     density = 10.98; %g/cm3, density of UO2
10    cp = 0.33; %J/(g K), specific heat of UO2
11    Ef = 3e-11; %J/s, energy released per fission
12    crosssection = 5.5e-22; %cm2, thermal crosssection for U-235
13    dens_U = 9.65; %g/cm3, density of U in UO2
14    q = 0.04; %Enrichment
15    Na = 6.022e23; %atoms/mol, Avagadro's number
16
17    %Reactor conditions
18    flux = 2.8e13; %n/(cm2 s), Neutron flux in the fuel
19    Ts = 685; %K, surface temperature of the pellet
20
21    %Pellet radius
22    Rf = 0.5; %cm
23    N = 100; %number of nodes along radius
24
25    %Time
26    tmax = 30; %seconds
27    M = 11; %number of time steps
28
```

The Command Window shows the following output:

```
>> rod_temp_profile_simple
>> rod_temp_profile_simple
>> rod_temp_profile_simple
>> rod_temp_profile_simple
>> rod_temp_profile_simple
fx >>
```

The Command Window also displays a table of values:

	0	3	6	9	12	15	18	21	24	27	30

The status bar at the bottom indicates the current file is `rod_temp_profile_simple` at line 8, column 27.



## Summary

- The Matlab function PDEPE solves partial differential equations in 1 spatial dimension and in time using implicit FEM
- You define the PDE you are solving by setting parameters using a function
- Other functions define the initial condition and the boundary conditions