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1 Introduction

In section 2 we present the heat equation. In section 3 we present the finite difference methode apply to heat equation.

2 Heat equation

The general heat equation is given by (y a-t-il une hypothèse simplificatrice amount supposant que ρ et c_p ne dépendent pas de la chaleur?):

$$\rho c_p \frac{\partial T(\mathbf{r}, t)}{\partial t} = \nabla \cdot [\lambda(\mathbf{r}) \nabla T(\mathbf{r}, t)] + \dot{q}_v, \quad (2.1)$$

where $\partial T(\mathbf{r}, t)$ is the temperature at postion \mathbf{r} and time t , ρ is the mass density of the material, c_p is the specific heat capacity, λ is the thermal conductivity (can also be denoted by κ) and \dot{q}_v is the volumetric heat source.

In the case of isotropic material ($\nabla \lambda(\mathbf{r}) = 0$) with no heat source we obtaine the whell know formula (phrase pourrie):

$$\frac{\partial T(\mathbf{r}, t)}{\partial t} = \alpha \Delta T(\mathbf{r}, t), \quad (2.2)$$

where $\alpha = \frac{\lambda}{\rho c_p}$ is the thermal diffusivity.

3 Finite difference scheme for heat equation

In this section, we present how to solve a heat problem numerically using a finite difference scheme depending on the space considered.

3.1 1D

In this section we present the 1D case of the heat equation for the Euler forward and backward scheme and the Crank-Nicolson scheme. We also describe the different boundary conditions and the case of an interface between two different materials.

Lets $T(x_i, t_l)$ be temperature at position x_i and time t_l , where the spatial step of discretization is Δx and the temporal step of discretization is Δt . In the following of this section, we note:

$$\gamma = \alpha \frac{\Delta t}{\Delta x^2}, \quad (3.1)$$

$$T_{i,l} = T(x_i, t_l), \quad (3.2)$$

and:

$$\dot{Q}_{i,l} = \rho c_p \dot{q}_v(x_i, t_l). \quad (3.3)$$

3.1.1 Euler forward

By including the forward time derivative expression A.4 and the half step second order space derivative A.10 in the heat equation 2.1 we obtaine the Euler forward scheme. Considering we are in an infinite homogeneous media, we have

$$\frac{T_{i,l+1} - T_{i,l}}{\Delta t} = \frac{\alpha}{\Delta x^2} [T_{i+1,l} + T_{i-1,l} - 2T_{i,l}] + \dot{Q}_{i,l}, \quad (3.4)$$

the volumetric heat source can also with postion and time. Hence we have

$$T_{i,l+1} = T_{i,l} + \gamma [T_{i+1,l} + T_{i-1,l} - 2T_{i,l}] + \dot{Q}_{i,j}. \quad (3.5)$$

The value of the temperature at step time t_{l+1} only depend on the value of the temperature at step t_l of the considered node and of it's direct neighbors. The variation of the temperature against time is easy to calculate with this scheme, we just have to know the temperature field at first step $t = 0$ (initial condition) the boundary condition at the border of the domain (at $x = 0$ and $x = x_{\max}$). The boundary conditions can be either constant temperture or constant flux... Different boundary conditions are presented in sections X to Y.

If we consider that the temperature at x_i is nearly the the mean value of the temperature of the neighbors points,

$$T(x_i, t_l) = T(x_{i+1}, t_l) + T(x_{i-1}, t_l) \quad (3.6)$$

and no volumetric heat source, the scheme converge if (nop, wrong)

$$\left| 1 + \alpha \frac{\Delta t}{\Delta x^2} \right| < 1 \quad (3.7)$$

then

$$\Delta t < \frac{2\Delta x^2}{\alpha} \quad (3.8)$$

3.1.2 Euler backward

By including the backward time derivative expression A.5 and the half step second order space derivative A.10 in the heat equation 2.1 we obtaine the Euler backward scheme. Considering we are in an infinite homogeneous media, we have

$$\frac{T_{i,l+1} - T_{i,l}}{\Delta t} = \frac{\alpha}{\Delta x^2} [T_{i+1,l+1} + T_{i-1,l+1} - 2T_{i,l+1}] + \dot{Q}_{i,l+1}, \quad (3.9)$$

and hence

$$T_{i,l+1} - \gamma [T_{i+1,l+1} + T_{i-1,l+1} - 2T_{i,l+1}] = T_{i,l} + \dot{Q}_{i,l+1}. \quad (3.10)$$

So for the Euleur bacward scheme one have to resolve a system of type

$$\mathbf{M}\mathbf{T}_{l+1} = \mathbf{T}_l, \quad (3.11)$$

This system can be resolved by different methods, but numerically the best way to do that in therms of time is a LU decomposition.

Consider a system with $N + 1$ node along x , with given boundary condition at x_0 and x_N , then eq. 3.10 lead to the system:

$$\begin{bmatrix} 1 + 2\gamma & -\gamma & 0 & 0 & \cdots \\ & \cdots & & & \\ \cdots & -\gamma & 1 + 2\gamma & -\gamma & \cdots \\ & & & \cdots & \\ \cdots & 0 & 0 & -\gamma & 1 + 2 - \gamma \end{bmatrix} \begin{pmatrix} T_{1,l+1} \\ \vdots \\ T_{i,l+1} \\ \vdots \\ T_{N-1,l+1} \end{pmatrix} = \begin{pmatrix} T_{1,l} + \dot{Q}_{1,l+1} + X_0 \\ \vdots \\ T_{i,l} + \dot{Q}_{i,l+1} \\ \vdots \\ T_{N-1,l} + \dot{Q}_{N-1,l} + X_N \end{pmatrix} \quad (3.12)$$

Where X_0 and X_N depend on the boundary conditions. This system can be resolved by different methods, but numerically the best way to do that in therms of time is a LU decomposition.

Eq. 3.12 can be rewrite under a more compact form:

$$\mathbf{D}(\gamma) \mathbf{T}_{i,l+1} = \mathbf{T}_{i,l} + \dot{\mathbf{Q}}_{i,l+1} + \mathbf{X}. \quad (3.13)$$

As for the simple implemenation presented in Appendix A, this scheme is absolutely convergent.

3.1.3 Crank-Nicolson

To obtained the Crank-Nicolson scheme we proceed as in A.2.3 and obtain

$$T_{i,l} + \frac{\gamma}{2} [T_{i-1,l} + T_{i+1,l} - 2T_{i,l}] + \frac{\dot{Q}_{i,l}}{2} = T_{i,l+1} - \frac{\gamma}{2} [T_{i-1,l+1} + T_{i+1,l+1} - 2T_{i,l+1}] + \frac{\dot{Q}_{i,l+1}}{2}, \quad (3.14)$$

that can be rewrite as

$$\mathbf{D} \left(\frac{\gamma}{2} \right) \mathbf{T}_{i,l+1} = \mathbf{D} \left(\frac{-\gamma}{2} \right) \mathbf{T}_{i,l} + \frac{\dot{\mathbf{Q}}_{i,l} + \dot{\mathbf{Q}}_{i,l+1}}{2} + \mathbf{X}. \quad (3.15)$$

3.1.4 Boundary conditions

Dirichlet boundary condition

A Dirichlet boundary condition is given by a constant temperature at one point, for example at node $i = 0$

$$T_{0,l} = T_0. \quad (3.16)$$

Neumann boundary condition

A Neumann boundary condition is given by a constant flux, for example the left flux at node $i = 0$:

$$\left. \frac{\partial T(x,t)}{\partial x} \right|_{x_0^-} = \partial T_0^-, \quad (3.17)$$

then the finite difference of the Laplacien is:

$$\left. \frac{\partial^2 T(x,t)}{\partial x^2} \right|_{x=x_0} = \frac{\partial T_0^-}{\Delta x} + \frac{T_{1,l} - T_{0,l}}{\Delta x^2} \quad (3.18)$$

Periodic boundary condition

A periodic boundary condition consist in considering an infinite medium along x with a periodicity of the length of the simulation. Then for $i \in [0; N]$, node 0 and node N are the same node then the finite difference of the Laplacien is:

$$\left. \frac{\partial^2 T(x,t)}{\partial x^2} \right|_{x=x_0} = \frac{T_{1,l} + T_{N-1,l} - 2T_{0,l}}{\Delta x^2}. \quad (3.19)$$

3.1.5 Interface between two different media

In the case where there are different media in the simulation, it is necessary to implement the case of an interface between two different media. To do that, we have to apply the finite difference method to

$$\nabla \cdot [\lambda(\mathbf{r}) \nabla T(\mathbf{r}, t)] \quad (3.20)$$

Let's consider an interface at $x_i = 0$, separating media 0 (for $x < x_i$) and 1 (for $x > x_i$). The thermal conductivity media m is noted λ^m , then expression 3.20 can be rewrite

$$\nabla \cdot [\lambda(\mathbf{r}) \nabla T(\mathbf{r}, t)] = \nabla \left[\lambda^1 \left. \frac{\partial T(\mathbf{r}, t)}{\partial x} \right|_{x_{i+1/2}} - \lambda^0 \left. \frac{\partial T(\mathbf{r}, t)}{\partial x} \right|_{x_{i-1/2}} \right] \quad (3.21)$$

then at time $t = t_l$

$$\nabla \cdot [\lambda(\mathbf{r}) \nabla T(\mathbf{r}, t)] = \frac{\lambda^0 T_{i-1,l} + \lambda^1 T_{i+1,l} - (\lambda^0 + \lambda^1) T_{i-1/2,l}}{\Delta x^2}. \quad (3.22)$$

In eq.3.22 it appears that node x_i behave like it's thermal properties are the mean value of the thermal properties of both media surrounding it.

A Finite difference

In this appendix, we show how to determine first and second order derivative from a discret function. Then we implement with a simple example different scheme of finite difference method.

A.1 Numerical derivation

A.1.1 First derivative

The finite difference methode (reference au livre sur la modelisation physique, voir comment ils l'introduise) is derive from the numerical derivation. Let $u(x)$ be a function of the variable x , where $u(x)$ and x are discret then the first order partial derivation is given by:

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i+} = \frac{u(x_{i+1}) - u(x_i)}{x_{i+1} - x_i}, \quad (\text{A.1})$$

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i-} = \frac{u(x_i) - u(x_{i-1})}{x_i - x_{i-1}}, \quad (\text{A.2})$$

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i\pm} = \frac{u(x_{i+1}) - u(x_{i-1})}{x_{i+1} - x_{i-1}}, \quad (\text{A.3})$$

where eq. A.1, A.2 and A.3 represente respectively the forward, backward and centered derivative. Considering constant step Δx for the discretisation of x , eq. A.1, to A.3 can be rewritten:

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i+} = \frac{u(x_{i+1}) - u(x_i)}{\Delta x}, \quad (\text{A.4})$$

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i-} = \frac{u(x_i) - u(x_{i-1})}{\Delta x}, \quad (\text{A.5})$$

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i\pm} = \frac{u(x_{i+1}) - u(x_{i-1})}{2\Delta x}, \quad (\text{A.6})$$

A.1.2 Second order derivative

The second derivative, considering full step first order derivative, is given by

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{\left. \frac{\partial u(x)}{\partial x} \right|_{x_{i+1}\pm} - \left. \frac{\partial u(x)}{\partial x} \right|_{x_{i-1}\pm}}{2\Delta x}, \quad (\text{A.7})$$

leading to

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{u(x_{i+2}) + u(x_{i-2}) - 2u(x_i)}{4\Delta x^2}. \quad (\text{A.8})$$

Here, the second order derivative depend on second neighbors, if we want that to depend on direct neighbors we have to make half-steps first order derivative

$$\left. \frac{\partial u(x)}{\partial x} \right|_{x_i\pm} = \frac{u(x_{i+1/2}) - u(x_{i-1/2})}{\Delta x}, \quad (\text{A.9})$$

which lead to

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{u(x_{i+1}) + u(x_{i-1}) - 2u(x_i)}{\Delta x^2}. \quad (\text{A.10})$$

A.2 Implementation

In this section we derived three finite difference schemes from a simple example to show how to implement these methods. Let consider the function

$$u(t) = e^{-\tau t}, \quad (\text{A.11})$$

then we this function respect

$$\frac{\partial u(t)}{\partial t} = -\tau u(t). \quad (\text{A.12})$$

Considering forward, backward or centered numerical derivative leads to different finite difference schemes, respectively Euler forward, Euler backward and Crank-Nicolson.

A.2.1 Euleur forward scheme

To resolve numerically the equation A.12 we use the forward derivative A.4 at time t_i :

$$\frac{u(t_{i+1}) - u(t_i)}{\Delta t} = -\tau u(t_i) \quad (\text{A.13})$$

that lead to

$$u(t_{i+1}) = (1 - \tau \Delta t) u(t_i). \quad (\text{A.14})$$

Then we see that we can determine the value of $u(t_i)$ if we know the value of $u(t)$ at previous step. This mean that we only need an initial value that will be consider the first step $u(t_0)$ to calculate the value of $u(t_i)$ for each i .

This scheme gives the value of $u(t_i)$ as a geomtrical serie (eq A.14), so if

$$|1 - \tau \Delta t| > 1, \quad (\text{A.15})$$

$u(t_i)$ will diverge: $|u(t_{i+1})| > |u(t_i)| \forall i$. Given that we search for a causal solution ($\Delta t > 0$), this scheme will give an oscillating non convergent solution ($u(t_{i+1}) = -u(t_i)$) if

$$\Delta t = \frac{2}{\tau}, \quad (\text{A.16})$$

and will converge if

$$\Delta t < \frac{2}{\tau}. \quad (\text{A.17})$$

A.2.2 Euler backward scheme

To resolve numerically the equation A.12 we use the backward derivative A.5 at time t_i :

$$\frac{u(t_i) - u(t_{i-1})}{\Delta t} = -\tau u(t_i) \quad (\text{A.18})$$

that lead to

$$u(t_i) = \frac{1}{1 + \tau \Delta t} u(t_{i-1}). \quad (\text{A.19})$$

With this example, as for the Euler forward scheme, if know the value of $u(t)$ at a given time (that will be define as the initial condition) we can calculate the value of $u(t_i)$ for each i .

Considering $\tau > 0$ and $\Delta t > 0$, this scheme allways converge.

A.2.3 Crank-Nicolson scheme

To resolve numerically the equation A.12 we use both the forward A.4 and backward A.5 derivation expression, considering a half time step. The Euler forward scheme A.14 gives:

$$u(t_{i+1/2}) = \left(1 - \frac{\tau\Delta t}{2}\right) u(t_i), \quad (\text{A.20})$$

the Euler backward scheme A.19 gives

$$u(t_{i+1-1/2}) = \left(1 + \frac{\tau\Delta t}{2}\right) u(t_{i+1}), \quad (\text{A.21})$$

and inserting A.21 into A.20 we obtain:

$$u(t_{i+1}) = \frac{2 - \tau\Delta t}{2 + \tau\Delta t} u(t_i). \quad (\text{A.22})$$

This scheme converge if

$$\left| \frac{2 - \tau\Delta t}{2 + \tau\Delta t} \right| < 1 \quad (\text{A.23})$$

wich is true $\forall \Delta t$ considering $\tau > 0$ and $\Delta t > 0$, so this scheme allways converge.