Contents

1 Introducion

In this document we present the software???

In section **??** we present the heat equation.

In section **??** we present the finite difference methode and application to heat equation.

2 Heat equation

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

$$\rho c_p \frac{\partial T(\mathbf{r}, t)}{\partial t} = \nabla \cdot [\lambda(\mathbf{r}) \nabla T(\mathbf{r}, t)] + \dot{q}_v, \tag{1}$$

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):

$$\frac{\partial T(\mathbf{r}, t)}{\partial t} = \alpha \Delta T(\mathbf{r}, t), \tag{2}$$

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

3 Finite difference scheme

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

3.1 1D

3.1.1 Euler forward

3.1.2 Euler backward

3.1.3 Crank-Nicolson

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:

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

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x_i-} = \frac{u(x_i) - u(x_{i-1})}{x_i - x_{i-1}}, \tag{4}$$

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x_i\pm} = \frac{u(x_{i+1}) - u(x_{i-1})}{x_{i+1} - x_{i-1}}, \tag{5}$$

where eq. 3, 4 and 5 represente respectively the forward, backward and centered derivative. Considering constant step Δx for the discretisation of x, eq. 3,to 5 can be rewriten:

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

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x_i-} = \frac{u(x_i) - u(x_{i-1})}{\Delta x}, \tag{7}$$

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x_i\pm} = \frac{u(x_{i+1}) - u(x_{i-1})}{2\Delta x}, \tag{8}$$

A.1.2 Second order derivative

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

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{\left.\frac{\partial u(x)}{\partial x}\right|_{x_{i+1}\pm} - \left.\frac{\partial u(x)}{\partial x}\right|_{x_{i-1}\pm}}{2\Delta x}, \tag{9}$$

leading to

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{u(x_{i+2}) + u(x_{i-2}) - 2u(x_i)}{4\,\Delta x^2}. \tag{10}$$

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

$$\left.\frac{\partial u(x)}{\partial x}\right|_{x_i\pm} = \frac{u\left(x_{i+1/2}\right) - u\left(x_{i-1/2}\right)}{\Delta x}, \tag{11}$$

which lead to

$$\frac{\partial^2 u(x)}{\partial x^2} = \frac{u(x_{i+1}) + u(x_{i-1}) - 2u(x_i)}{\Delta x^2}. \tag{12}$$

A.2 Method

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

$$u(t) = \mathrm{e}^{-\tau t}, \tag{13}$$

then we this function respect

$$\frac{\partial u(t)}{\partial t} = -\tau u(t). \tag{14}$$

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 14 we use the forward derivative 6 at time t_i:

$$\frac{u(t_{i+1}) - u(t_i)}{\Delta t} = -\tau u(t_i) \tag{15}$$

that lead to

$$u(t_{i+1}) = (1 - \tau \Delta t)\, u(t_i). \tag{16}$$

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 16), so if

$$|(1 - \tau \Delta t| > 1, \tag{17}$$

$u(t_i)$ will diverge: $|u(t_{i+1})| > |u(t_{i+1})| \, \forall i$. 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

$$\Delta t = \frac{2}{\tau}, \tag{18}$$

and will converge if

$$\Delta t < \frac{2}{\tau}. \tag{19}$$

A.2.2 Euler backward scheme

To resolve numerically the equation 14 we use the backward derivative 7 at time t_i:

$$\frac{u(t_i) - u(t_{i-1})}{\Delta t} = -\tau u(t_i) \tag{20}$$

that lead to

$$u(t_i) = \frac{1}{1 + \tau \Delta t} u(t_{i-1}). \tag{21}$$

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 14 we use both the forward 6 and backward 7 derivation expression, considering a half time step. The Euler forward scheme 16 gives:

$$u\left(t_{i+1/2}\right) = \left(1 - \frac{\tau \Delta t}{2}\right) u\left(t_i\right), \tag{22}$$

the Euler backward scheme 21 gives

$$u\left(t_{i+1-1/2}\right) = \left(1 + \frac{\tau \Delta t}{2}\right) u\left(t_{i+1}\right), \tag{23}$$

and inserting 23 into 22 we obtain:

$$u\left(t_{i+1}\right) = \frac{2 - \tau \Delta t}{2 + \tau \Delta t} u\left(t_i\right). \tag{24}$$

This scheme converge if

$$\left|\frac{2 - \tau \Delta t}{2 + \tau \Delta t}\right| < 1 \tag{25}$$

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