HAMT - Tool for simulation of Heat And Mass Transfer

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Contents

1 Numerics

1.1 Finite Difference Method - FDM

First order Discritization.

$$f'_f = \frac{f_{i+1} - f_i}{\Delta x} \tag{1.1}$$

$$f'_b = \frac{f_i - f_{i-1}}{\Delta x} \tag{1.2}$$

$$f'_c = \frac{1}{2}\left(f'_f + f'_b\right) = \frac{1}{2}\left(\frac{f_{i+1} - f_i}{\Delta x} + \frac{f_i - f_{i-1}}{\Delta x}\right) = \frac{f_{i+1} - f_{i-1}}{2\,\Delta x} \tag{1.3}$$

second order

$$f'' = \frac{f'_f - f'_b}{\Delta x} = \frac{f_{i+1} - f_i}{\Delta x^2} - \frac{f_i - f_{i-1}}{\Delta x^2} = \frac{f_{i+1} - 2\,f_i + f_{i-1}}{\Delta x^2} \tag{1.4}$$

Assuming the differentials $a\,\frac{\partial f}{\partial x}$ and $a\,\frac{\partial^2 f}{\partial x^2}$ where a is not constant.

$$a\,f'_c = \frac{1}{2}\left(\frac{a_{i+1}(f_{i+1} - f_i)}{\Delta x} + \frac{a_{i-1}(f_i - f_{i-1})}{\Delta x}\right) = \frac{a_{i+1}f_{i+1} + (a_{i-1} - a_{i+1})f_i - a_{i-1}f_{i-1}}{2\,\Delta x} \tag{1.5}$$

$$a\,f'' = a_{i+1}\frac{f_{i+1} - f_i}{\Delta x^2} - a_{i-1}\frac{f_i - f_{i-1}}{\Delta x^2} = \frac{a_{i+1}f_{i+1} - (a_{i+1} + a_{i-1})f_i + a_{i-1}f_{i-1}}{\Delta x^2} \tag{1.6}$$

1.1.1 Dirichlet Boundary Conditions

$$f|_i = f_0 \tag{1.7}$$

1.1.2 Neumann Boundary Conditions

$$\left.\frac{\partial f}{\partial x}\right|_{x=i} = c \tag{1.8}$$

$$\frac{f_i - fi - i}{\Delta x} = c \tag{1.9}$$

$$f_i - f_{i-i} = \Delta x\,c \tag{1.10}$$

1.1.3 Radiation Boundary Conditions

$$\vec{q_r} = \epsilon\,\sigma\,T^4\,\vec{n} \tag{1.11}$$

Using the Taylor series

$$\mathrm{T}\,f(x;a) = \sum_{n=0}^{\infty}\frac{f^{(n)}(a)}{n!}(x-a)^n \tag{1.12}$$

we get the linearized equation for the heat flux due to radiation

$$\mathrm{T}\,\dot{q}_r(T;T_0) = (4\,\epsilon\,\sigma\,T_0^3)T - 3\,\epsilon\,\sigma\,T_0^4. \tag{1.13}$$

Using eqation (2.3)

$$-\lambda\frac{\partial T}{\partial x} = \mathrm{T}\,\dot{q}_r(T;T_0) \tag{1.14}$$

leads to the discitized, linear equation

$$\left(1 + 4\,k\,T_0^3\right)T_i - T_{i-1} = 3\,k\,T_0^4 \tag{1.15}$$

where

$$k = \frac{\epsilon\,\sigma\,\Delta x}{\lambda} \tag{1.16}$$

2 Heat Transfer

The base equation for the heat transfer is the balance equation of the form

$$\frac{\partial \rho}{\partial t} + \nabla \vec{j} = f(\vec{r}, t) \tag{2.1}$$

where ρ is the density of the quantity in question, $\vec{j}$ is the flux, $\vec{r}$ is the position vector and t is time. For heat transfer problem we define ρ as the volumetric heat density q which is defined as

$$q = \frac{Q}{V} = c\,\rho\,T \tag{2.2}$$

$\vec{j}$ is equvalent to the heat flux $\vec{\dot{q}}$

$$\vec{\dot{q}} = -\lambda\,\nabla T \tag{2.3}$$

and the source$f(\vec{r}, t)$ is the volumetrix heat source $\dot{q}_v(\vec{r}, t)$. Inserting 2.2 and 2.3 in 2.1 leads to the heat transfer equation

$$\frac{\partial (c\,\rho\,T)}{\partial t} + \nabla(-\lambda\,\nabla T) = \dot{q}_v(\vec{r}, t) \tag{2.4}$$

where the quantities are defined as seen in table **??**.

Table 2.1: Electron beam - simulation parameters

Quantitiy	Description	Unit
c	Specific heat capacity	$\mathrm{J\,kg^{-1}\,K^{-1}}$
ρ	Density	$\mathrm{kg\,m^{-3}}$
T	Temperature	K
λ	Thermal conductivity	$\mathrm{W\,m^{-1}\,K^{-1}}$
$\dot{q}_v$	Volumetric heat source	$\mathrm{W\,m^{-3}}$

2.1 Homogeneous Heat Transfer Equation

Aussuming...

$$\lambda\,\Delta T = 0 \tag{2.5}$$

The homogeneous heat equation in cartesian coordinates is expressed as

$$\lambda\frac{\partial^2 T}{\partial x^2} + \lambda\frac{\partial^2 T}{\partial y^2} + \lambda\frac{\partial^2 T}{\partial z^2} = 0 \tag{2.6}$$

while in cylinder coordinates as

$$\lambda\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \lambda\frac{1}{r^2}\frac{\partial^2 T}{\partial \phi^2} + \lambda\frac{\partial^2 T}{\partial z^2} = 0. \tag{2.7}$$

2.2 FDM - Homogeneous Equidistant Cartesian 2D

By assuming only the x and y directions equation (2.6) reduces to

$$\lambda\frac{\partial^2 T}{\partial x^2} + \lambda\frac{\partial^2 T}{\partial y^2} = 0. \tag{2.8}$$

2.2.1 Central Equation

Using equation (1.6) equation (2.8) can be discritizised as

$$\lambda_{i+1,j}T_{i+1,j} + \lambda_{i,j+1}T_{i,j+1} - \lambda_{tot}T_{i,j} + \lambda_{i-1,j}T_{i-1,j} + \lambda_{i,j-1}T_{i,j-1} = 0 \tag{2.9}$$

where

$$\lambda_{tot} = \lambda_{i+1,j} + \lambda_{i-1,j} + \lambda_{i,j+1} + \lambda_{i,j-1}. \tag{2.10}$$

In case any of the λ paramters is to be taken on a boundary between two segments, a mean between to is to take. The correctness of this assumptions can be proven by setting up 4 equations around a center node using Fourrier's law. For $\lambda = const$ the equation reduces to

$$T_{i+1,j} + T_{i,j+1} - 4\,T_{i,j} + T_{i-1,j} + T_{i,j-1} = 0 \tag{2.11}$$

2.2.2 Corner Equations

2.2.3 Side Equations

2.2.4 Verification