HAMT - Tool for simulation of Heat And Mass Transfer

Leo Basov

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Contents

1 Numerics

According to [1] the Gaus divergenze theorem can be rewritten as

$$\int_V \nabla \vec{F} \; \mathrm{d}^n V = \oint_S \vec{F} \cdot \vec{n} \; \mathrm{d}^{n-1} S \tag{1.1}$$

Using ∇f for $\vec{f}$ Eqn. (1.1) can be rewritten as

$$\int_V \nabla^2 f \; \mathrm{d}^n V = \oint_S (\nabla f) \cdot \vec{n} \; \mathrm{d}^{n-1} S \tag{1.2}$$

For the numerical solution a cell wise desrcitization is made. Assuming that $\nabla^2 f$ is constants over a cell the equation above reduces to

$$V_C \cdot \nabla^2 f = \sum_i^N (\nabla f) \cdot \vec{n}_i \cdot S_i. \tag{1.3}$$

1.1 Gradient

The base equation is given as

$$\int_A \nabla f \, \mathrm{d}A = \oint_S f \cdot \vec{n} \, \mathrm{d}S \tag{1.4}$$

The left hand side of the equation can be rewritten as

$$\int_A \nabla f \, \mathrm{d}A = A_c \cdot \nabla f_c \tag{1.5}$$

The right hand side can be written as

$$\oint_S f \cdot \vec{n} \, \mathrm{d}S = \sum_{i=1}^N \frac{f_{i+1} + f_i}{2} \cdot \vec{n}_i \cdot |\vec{r}_{i+1,i}| \tag{1.6}$$

where $\vec{r}_{i+1,i} = \vec{x}_{i+1} - \vec{x}_i$ and it can be written

$$\vec{n}_i \cdot |\vec{r}_{i+1,i}| = M_{rot} \cdot \vec{r}_{i+1,i} \tag{1.7}$$

where

$$M_{rot} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1.8}$$

with $\theta = -\pi/2$

$$M_{rot} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1.9}$$

Since the integral mus be performed over a closed loop

$$\begin{aligned} \nabla f_c &= \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^N (f_{i+1} + f_i) \cdot M \cdot \vec{r}_{i+1,i} \\ &= \frac{1}{2 \cdot A_c} \cdot [(f_{i+1} + f_i) \cdot M \cdot (\vec{x}_{i+1} - \vec{x}_i) + \dots + (f_i + f_{i-1}) \cdot M \cdot \vec{x}_i - \vec{x}_{i-1}] \\ &= \frac{1}{2 \cdot A_c} \cdot [f_i \cdot M \cdot (\vec{x}_{i+1} - \vec{x}_{i-1}) + f_{i+1} \cdot M \cdot (\vec{x}_{i+2} - \vec{x}_i) + \dots] \end{aligned} \tag{1.10}$$

Thus

$$\nabla f_c = \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^{N} f_i \cdot M \cdot \vec{r}_{i+1,i-1} \tag{1.11}$$

1.2 Normal derivative

For the normal derivative at the cell wall w with the normal vector n_w one can write

$$\underbrace{\nabla f_c \cdot \vec{n}_w}_{\nabla_w f_c} = \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^{N} f_i \cdot (M \cdot \vec{r}_{i+1,i-1}) \cdot \vec{n}_w \tag{1.12}$$

To find the derivative on a node surrounded by K neighbouring cells with the total surface $A_{tot} = \sum_{c=1}^{K} A_c$

$$\sum_{c=1}^{K} \frac{A_c}{A_{tot}} \cdot \nabla_{c,w} f_c = \sum_{c=1}^{K} \frac{A_c}{A_{tot}} \cdot \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^{N} f_{c,i} \cdot (M \cdot \vec{r}_{c,i+1,i-1}) \cdot \vec{n}_{c,w} \tag{1.13}$$

using $\overline{A_c} = \frac{A_c}{A_{tot}}$

$$\sum_{c=1}^{K} \overline{A_c} \cdot \nabla_{c,w} f_c = \frac{1}{2 \cdot A_{tot}} \cdot \sum_{c=1}^{K} \sum_{i=1}^{N} f_{c,i} \cdot (M \cdot \vec{r}_{c,i+1,i-1}) \cdot \vec{n}_{c,w} \tag{1.14}$$

1.3 Laplace

The integral is made over a pseudo cell which connects the barycentres of adjacent cells

$$\begin{aligned} \nabla^2 f \cdot \underbrace{\sum_{b=1}^{N} A_b}_{A_{b,tot}} &= \sum_{b=1}^{N} \nabla f \cdot M \cdot \vec{r}_{b+1,b} \\ &= \sum_{b=1}^{N} \frac{A_b \cdot \nabla f_b + A_{b+1} \cdot \nabla f_{b+1}}{A_{b+1,b}} \cdot M \cdot \vec{r}_{b+1,b} \end{aligned} \tag{1.15}$$

Using Eqn. (1.11)

$$\nabla^2 f \cdot A_{b,tot} = \sum_{b=1}^{N} \frac{1}{2 \cdot A_{b+1,b}} \cdot \left(\sum_{q=0}^{1} \sum_{i=1}^{3} f_i^{b+q} \cdot M \cdot \vec{r}_{i+1,i-1}^{\,b+q} \right) \cdot M \cdot \vec{r}_{b+1,b} \tag{1.16}$$

As the gradient is considered constant inside the cell

$$\nabla^2 f \approx \frac{1}{2 \cdot A_{b,tot}} \cdot \sum_{b=1}^{N} \frac{1}{A_{b+1,b}} \cdot \left(\sum_{q=0}^{1} \sum_{i=1}^{3} f_i^{b+q} \cdot M \cdot \vec{r}_{i+1,i-1}^{\,b+q} \right) \cdot M \cdot \vec{r}_{b+1,b} \tag{1.17}$$

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 2.1.

Table 2.1: Heat Transfer - 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 no time dependance $\frac{\partial(c\,\rho\,T)}{\partial t} = 0$ and no heat source $\dot{q}_v(\vec{r}, t) = 0$ Eqn. (2.4) reduces to

$$\nabla(\lambda\,\nabla T) = 0 \tag{2.5}$$

where $\lambda = \mathrm{fn}(\vec{r})$. According to the prodcut rules for vector calculus Eqn. (2.5) evaluates to

$$\nabla(\lambda\,\nabla T) = \nabla T \cdot (\nabla \lambda) + \lambda\,(\nabla \cdot \nabla T) \tag{2.6}$$

$$\nabla(\lambda\,\nabla T) = \nabla \lambda \cdot \nabla T + \lambda \cdot \nabla^2 T \tag{2.7}$$

which leads to

$$\nabla \lambda \cdot \nabla T + \lambda \cdot \nabla^2 T = 0. \tag{2.8}$$

2.1.1 2D Cartesian Formulation

Evaluating Eq. (2.5) for two variables in cartesian form leads to

$$
\begin{aligned}
\nabla(\lambda\,\nabla T) &= \frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right) && (2.9)\\
&= \frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x} + \lambda\frac{\partial^2 T}{\partial x^2} + \frac{\partial \lambda}{\partial y}\frac{\partial T}{\partial y} + \lambda\frac{\partial^2 T}{\partial y^2} && (2.10)\\
&= \frac{\partial \lambda}{\partial x}\frac{\partial T}{\partial x} + \frac{\partial \lambda}{\partial y}\frac{\partial T}{\partial y} + \lambda\frac{\partial^2 T}{\partial x^2} + \lambda\frac{\partial^2 T}{\partial y^2} && (2.11)\\
&= \nabla\lambda\cdot\nabla T + \lambda\cdot\nabla^2 T && (2.12)
\end{aligned}
$$

2.1.2 2D Cylindrical Formulation

Evaluating Eq. (2.5) for two variables in cartesian form leads to

$$
\begin{aligned}
\nabla(\lambda\,\nabla T) &= \frac{\partial}{\partial r}\left(\lambda\frac{\partial T}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial \phi}\left(\lambda\frac{1}{r}\frac{\partial T}{\partial \phi}\right) && (2.13)\\
&= \frac{\partial \lambda}{\partial r}\frac{\partial T}{\partial r} + \lambda\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\left[\frac{\partial \lambda}{\partial \phi}\frac{1}{r}\frac{\partial T}{\partial \phi} + \lambda\frac{1}{r}\frac{\partial^2 T}{\partial \phi^2}\right] && (2.14)\\
&= \frac{\partial \lambda}{\partial r}\frac{\partial T}{\partial r} + \frac{1}{r}\frac{\partial \lambda}{\partial \phi}\frac{1}{r}\frac{\partial T}{\partial \phi} + \lambda\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \phi^2}\right] && (2.15)\\
&= \nabla\lambda\cdot\nabla T + \lambda\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \phi^2}\right] && (2.16)
\end{aligned}
$$

2.2 Finite-Difference Scheme - Triangular Unordered 2D Grid

Using a second order Taylor serias expansion around a arbitray point in space for two variables on can write

$$
\mathrm{T}\, f(x;a) = f(a) + \sum_{j=1}^{2}\frac{\partial f(a)}{\partial x_j} + \frac{1}{2}\sum_{j=1}^{2}\sum_{k=1}^{2}\frac{\partial^2 f(a)}{\partial x_j \partial x_k}(x_k - a_k) + O(\Delta^3) \qquad (2.17)
$$

2.3 Finite-Difference Scheme - Homogeneous Equidistant 2D Grid

2.3.1 Boundary Conditions

For all boundary condition is present the dirichlet boundary condtions always orride other boudnary conditions on contact nodes. If two cells with different dirichlet boundary condtions touch, a arichmetical mean is taken.

Corner Boundary Conditions

Examples buttom left corner

$$
\begin{aligned}
T_{i+1,j} - T_{i,j} &= \Delta x_1\, c_1 && (2.18)\\
T_{i,j+1} - T_{i,j} &= \Delta x_2\, c_2 && (2.19)
\end{aligned}
$$

By adding the two functions one gets

$$
T_{i+1,j} + T_{i,j+1} - 2T_{i,j} = \Delta x_1\, c_1 + \Delta x_2\, c_2. \qquad (2.20)
$$

Radiation Boundary Conditions

$$\vec{\dot{q}_r} = \epsilon\,\sigma\,T^4\,\vec{n} \tag{2.21}$$

Using the Taylor series

$$\mathrm{T}\,f(x;a) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n \tag{2.22}$$

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

$$\mathrm{T}\,\dot{q}_r(T;T_0) = (4\,\epsilon\,\sigma\,T_0^3)T - 3\,\epsilon\,\sigma\,T_0^4. \tag{2.23}$$

Using eqation (2.3)

$$-\lambda\frac{\partial T}{\partial x} = \mathrm{T}\,\dot{q}_r(T;T_0) \tag{2.24}$$

leads to the discitized, linear equation

$$\left(1 + 4\,k\,T_0^3\right)T_i - T_{i-1} = 3\,k\,T_0^4 \tag{2.25}$$

where

$$k = \frac{\epsilon\,\sigma\,\Delta x}{\lambda} \tag{2.26}$$

Table 2.2: Radiation Boundary Condition - parameters

Quantitiy	Description	Unit
ϵ	Emissivity factor	$-$
σ	Stefan-Boltzmann constant	$\mathrm{W\,m^{-2}\,K^{-4}}$
Δx	Spatial step	m

2.3.2 Cartesian Coordinates

The homogeneous heat equation in cartesian coordinates is expressed as

$$\lambda\frac{\partial^2 T}{\partial x^2} + \lambda\frac{\partial^2 T}{\partial y^2} + \lambda\frac{\partial^2 T}{\partial z^2} = 0 \tag{2.27}$$

By assuming only the x and y directions equation (2.27) reduces to

$$\lambda\frac{\partial^2 T}{\partial x^2} + \lambda\frac{\partial^2 T}{\partial y^2} = 0. \tag{2.28}$$

Using equation (**??**) equation (2.28) can be discritizised as

$$\lambda_{i+1,j}T_{i+1,j} + \lambda_{i,j+1}T_{i,j+1} - \lambda_{tot}T_{i,j} + \lambda_{i-1,j}T_{i-1,j} + \lambda_{i,j-1}T_{i,j-1} = 0 \tag{2.29}$$

where

$$\lambda_{tot} = \lambda_{i+1,j} + \lambda_{i-1,j} + \lambda_{i,j+1} + \lambda_{i,j-1}. \tag{2.30}$$

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

$$T_{i+1,j} + T_{i,j+1} - 4\,T_{i,j} + T_{i-1,j} + T_{i,j-1} = 0 \tag{2.31}$$

2.3.3 Cylinder Coordinates

while in cylinder coordinates as

$$\lambda \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) + \lambda \frac{1}{r^2} \frac{\partial^2 T}{\partial \phi^2} + \lambda \frac{\partial^2 T}{\partial z^2} = 0. \tag{2.32}$$

2.3.4 Verification

Heat codnuctivity trhough a layerd wall

$$\dot{q} = \left(\sum_{i=1}^{N} \frac{\Delta x_i}{\lambda_i} \right)^{-1} \Delta T \tag{2.33}$$

Bibliography

[1] G Erlebacher. "Finite difference operators on unstructured triangular meshes". In: *The Free-Lagrange Method*. Springer, 1985, pp. 22–53.