HAMT - Tool for simulation of Heat And Mass Transfer

Leo Basov

March 20, 2022

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

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

1.1 2D Application for triangular mesh

For a trinagular mesh assuming one can write

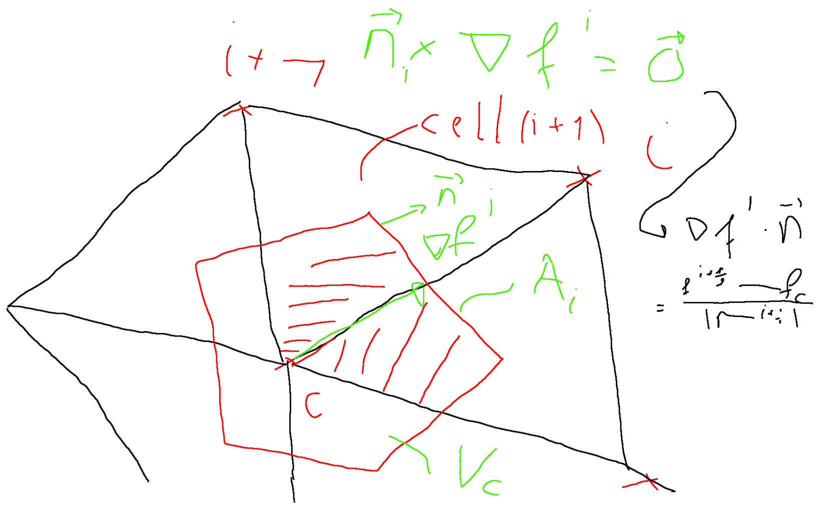

Figure 1.1: Test

$$\nabla f \cdot \vec{n}_i = \frac{f_i - f_C}{|\vec{r}_i|} \tag{1.4}$$

for a 2d geometriy $A_{C,i}$ becomes a line segment

$$A_i = |\vec{b}_{i+1} - \vec{b}_i| = L_i \tag{1.5}$$

where $\vec{b}_i$ is the barycentre of the last cell containing the point i. In this context V_C becomes the volume of created new cell A_C which is defined as

$$A_C = \frac{1}{2} \cdot \sum_{i}^{N} \vec{b}_{i+1} \times \vec{b}_i \tag{1.6}$$

This leads to

$$\nabla^2 f = \frac{1}{A_C} \cdot \sum_{i}^{N} \frac{f_i - f_C}{|\vec{r}_i|} \cdot |\vec{b}_{i+1} - \vec{b}_i|. \tag{1.7}$$

1.2 Gradient

Is given as

$$\nabla f_c = \frac{1}{2A_c} \sum_{i=1}^{3} f_i \cdot \begin{bmatrix} -e_{i,y} \\ e_{i,x} \\ e_{i,z} \end{bmatrix} \tag{1.8}$$

where $\vec{e}_i$ is the vector reptreseting the ith vertex and is rotated to point to the cell centre and f_i is the function value at the vertix i.

$$f_i = \frac{1}{2} \cdot (f_{i,0} + f_{i,1}) \tag{1.9}$$

where $f_{i,k}$ is the value of the kth node of the vertex.

$$\vec{e}_i = \vec{e}_{i,1} - \vec{e}_{i,0} \tag{1.10}$$

Leads to

$$\nabla f_c = \frac{1}{4A_c} \sum_{k=2}^{3} \left((f_k + f_{k-1}) \cdot \begin{bmatrix} -(\vec{x}_k - \vec{x}_{k-1})_y \\ (\vec{x}_k - \vec{x}_{k-1})_x \\ (\vec{x}_k - \vec{x}_{k-1})_z \end{bmatrix} \right) \tag{1.11}$$

The derevative at given point p sorounded by cells is given as

$$\nabla f_p = \frac{1}{\sum_{c=1}^{N} A_c} \cdot \sum_{c=1}^{N} \nabla f_c \cdot A_c \tag{1.12}$$

since we are only interested in the normal derivative at point p

$$|\nabla f_p|_{\vec{n}_p} = \frac{1}{\sum_{c=1}^{N} A_c} \cdot \sum_{c=1}^{N} \nabla f_c \cdot \vec{n}_p \cdot A_c \tag{1.13}$$

1.3 Gradient 2

Eqn. (1.1)

$$\int_V \vec{c} \cdot \nabla f \; \mathrm{d}^n V = \oint_S \vec{c} f \cdot \vec{n} \; \mathrm{d}^{n-1} S + \underbrace{\int_V f (\nabla \cdot \vec{c}) \; \mathrm{d}^n V}_{=0 \text{ for } \vec{c}=const} \tag{1.14}$$

interpreting $\vec{c}$ as the normal of the wall at which the gradient is given ($\vec{n}_g$) leads to

$$\int_V \nabla_{\vec{n}_g} f \; \mathrm{d}^n V = \oint_S f \cdot (\vec{n}_g \cdot \vec{n}) \; \mathrm{d}^{n-1} S \tag{1.15}$$

Discritezising over a cell and assuming const $\nabla_{\vec{n}_g} f$ over cell leads to

$$A_c \cdot \nabla_{\vec{n}_g} f = \sum_{i=1}^{3} \frac{1}{2} \cdot (f_{i+1} + f_i) \cdot (\vec{n}_g \cdot \underbrace{\vec{n}_i \cdot S_i}_{M \cdot (\vec{x}_{i+1} - \vec{x}_i)}) \tag{1.16}$$

within

$$\vec{r}_{i+1,i} = \vec{x}_{i+1} - \vec{x}_i \tag{1.17}$$

and

$$M = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{1.18}$$

is

$$M \cdot \vec{r}_{i+1,i} = \begin{bmatrix} r_{i+1,i,y} \\ -r_{i+1,i,x} \\ r_{i+1,i,z} \end{bmatrix} = \vec{p}_{i+1,i} \tag{1.19}$$

leads to

$$\nabla_{\vec{n}_g} f = \sum_{i=1}^{2} \frac{f_{i+1} + f_i}{2A_c} \cdot \vec{n}_g \cdot \vec{p}_{i+1,i} + \frac{f_1 + f_3}{2A_c} \cdot \vec{n}_g \cdot \vec{p}_{1,3} \tag{1.20}$$

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

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

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

$$T_{i+1,j} - T_{i,j} = \Delta x_1\, c_1 \tag{2.18}$$

$$T_{i,j+1} - T_{i,j} = \Delta x_2\, c_2 \tag{2.19}$$

By adding the two functions one gets

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

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.