

Discretization of a triangular Grid

Leo Basov

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1 Cartesian Coordinates

1.1 Gradient

The base equation is given as

$$\int_A \nabla f \, dA = \oint_S f \cdot \vec{n} \, dS \quad (1.1)$$

The left hand side of the equation can be rewritten as

$$\int_A \nabla f \, dA = A_c \cdot \nabla f_c \quad (1.2)$$

The right hand side can be written as

$$\oint_S f \cdot \vec{n} \, dS = \sum_{i=1}^N \frac{f_{i+1} + f_i}{2} \cdot \vec{n}_i \cdot |\vec{r}_{i+1,i}| \quad (1.3)$$

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

$$\vec{n}_i \cdot |\vec{r}_{i+1,i}| = M_{rot} \cdot \vec{r}_{i+1,i} \quad (1.4)$$

where

$$M_{rot} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (1.5)$$

with $\theta = -\pi/2$

$$M_{rot} = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (1.6)$$

Since the integral mus be performed over a closed loop

$$\begin{aligned} \nabla f_c &= \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^N (f_{i+1} + f_i) \cdot M \cdot \vec{r}_{i+1,i} \\ &= \frac{1}{2 \cdot A_c} \cdot [(f_{i+1} + f_i) \cdot M \cdot (\vec{x}_{i+1} - \vec{x}_i) + \dots + (f_i + f_{i-1}) \cdot M \cdot \vec{x}_i - \vec{x}_{i-1}] \\ &= \frac{1}{2 \cdot A_c} \cdot [f_i \cdot M \cdot (\vec{x}_{i+1} - \vec{x}_{i-1}) + f_{i+1} \cdot M \cdot (\vec{x}_{i+2} - \vec{x}_i) + \dots] \end{aligned} \quad (1.7)$$

Thus

$$\nabla f_c = \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^N f_i \cdot M \cdot \vec{r}_{i+1,i-1} \quad (1.8)$$

1.2 Normal derivative

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

$$\underbrace{\nabla f_c \cdot \vec{n}_w}_{\nabla_w f_c} = \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^N f_i \cdot (M \cdot \vec{r}_{i+1,i-1}) \cdot \vec{n}_w \quad (1.9)$$

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

$$\sum_{c=1}^K \frac{A_c}{A_{tot}} \cdot \nabla_{c,w} f_c = \sum_{c=1}^K \frac{A_c}{A_{tot}} \cdot \frac{1}{2 \cdot A_c} \cdot \sum_{i=1}^N f_{c,i} \cdot (M \cdot \vec{r}_{c,i+1,i-1}) \cdot \vec{n}_{c,w} \quad (1.10)$$

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

$$\sum_{c=1}^K \overline{A_c} \cdot \nabla_{c,w} f_c = \frac{1}{2 \cdot A_{tot}} \cdot \sum_{c=1}^K \sum_{i=1}^N f_{c,i} \cdot (M \cdot \vec{r}_{c,i+1,i-1}) \cdot \vec{n}_{c,w} \quad (1.11)$$

1.3 Laplace

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

$$\begin{aligned} \nabla^2 f \cdot \underbrace{\sum_{b=1}^N A_b}_{A_{b,tot}} &= \sum_{b=1}^N \nabla f \cdot M \cdot \vec{r}_{b+1,b} \\ &= \sum_{b=1}^N \frac{A_b \cdot \nabla f_b + A_{b+1} \cdot \nabla f_{b+1}}{A_{b+1,b}} \cdot M \cdot \vec{r}_{b+1,b} \end{aligned} \quad (1.12)$$

Using Eqn. (1.8)

$$\nabla^2 f \cdot A_{b,tot} = \sum_{b=1}^N \frac{1}{2 \cdot A_{b+1,b}} \cdot \left(\sum_{q=0}^1 \sum_{i=1}^3 f_i^{b+q} \cdot M \cdot \vec{r}_{i+1,i-1}^{b+q} \right) \cdot M \cdot \vec{r}_{b+1,b} \quad (1.13)$$

As the gradient is considered constant inside the cell

$$\nabla^2 f \approx \frac{1}{2 \cdot A_{b,tot}} \cdot \sum_{b=1}^N \frac{1}{A_{b+1,b}} \cdot \left(\sum_{q=0}^1 \sum_{i=1}^3 f_i^{b+q} \cdot M \cdot \vec{r}_{i+1,i-1}^{b+q} \right) \cdot M \cdot \vec{r}_{b+1,b} \quad (1.14)$$

2 Cylindrical Coordinates

2.1 Gradient

The base equation is given as

$$\int_V \nabla f \, dV = \oint_S f \cdot \vec{n} \, dS \quad (2.1)$$

2.2 Left hand side

The left hand side of the equation above can be expressed as follows

$$\int_V \nabla f \, dV = \iiint \nabla f \, dx dy dz \quad (2.2)$$

For a coordinate transformation first consider the Cartesian coordinates in cylindrical

$$x = r \cos \theta \quad (2.3)$$

$$y = r \sin \theta \quad (2.4)$$

$$z = z \quad (2.5)$$

For a 2d case the Jacobian can be expressed as

$$J = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial z} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial z} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial z} \end{pmatrix} = \begin{pmatrix} \cos \theta & -r \sin \theta & 0 \\ \sin \theta & r \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.6)$$

with the determinant

$$\det(J) = r \quad (2.7)$$

Using this information the left hand side can be expressed in cylindrical coordinates as

$$\iiint \nabla f \, dx dy dz = \iiint \nabla f \cdot r \, dr d\theta dz \quad (2.8)$$

For further calculations $\frac{\partial}{\partial \theta}$ and ∇f to be constant over a cell hence

$$\iiint \nabla f \cdot r \, dr d\theta dz = \nabla f \cdot 2\pi \cdot \iint r \, dr dz \quad (2.9)$$

Assuming that the the point of interest is surrounded by a polygonal cell which consists of sub cells, the integral can be expressed as a sum of integrals over the sub cells:

$$\nabla f \cdot 2\pi \cdot \iint r \, dr dz = \nabla f \cdot 2\pi \cdot \sum_{i=1}^N \iint_{p_{i,0}}^{p_{i,1}(r,z)} r \, dr dz. \quad (2.10)$$

2.2.1 Triangular Mesh

To solve the equation on a cell of a triangular mesh the equation is first solved on a unit triangle. The solution on a unit triangle is the special case of the solution on a right triangle:

$$\nabla f \cdot 2\pi \cdot \int_{z_0}^{z_1} \int_{r_1}^{r(z)} r \, dr dz = \nabla f \cdot 2\pi \cdot \int_0^1 \int_0^{1-z} r \, dr dz. \quad (2.11)$$

To solve the equation on an arbitrary triangle

$$\iint r \, dr dz = \int_0^1 \int_0^{1-\tilde{z}} \tilde{r}(r(\tilde{r}, \tilde{z}), z(\tilde{r}, \tilde{z})) |\det(J)| \, d\tilde{r} d\tilde{z}. \quad (2.12)$$

Assuming that the vertices of the original triangle are denoted \mathbf{a} , \mathbf{b} and \mathbf{c} the map can be defined as

$$\mathbf{g}: (u, v) \mapsto \mathbf{a} + u(\mathbf{b} - \mathbf{a}) + v(\mathbf{c} - \mathbf{a}) \quad (2.13)$$

which for our case means

$$r(\tilde{r}, \tilde{z}) = a_r + \tilde{r}(b_r - a_r) + \tilde{z}(c_r - a_r) \quad (2.14)$$

and the determinant of the Jacobian is constant as

$$\det(J) = (b_r - a_r)(c_z - a_z) - (c_r - a_r)(b_z - a_z). \quad (2.15)$$

The equation can now be rewritten to

$$\iint r \, dr dz = |\det(J)| \int_0^1 \int_0^{1-\tilde{z}} \tilde{r}(\tilde{r}, \tilde{z}) \, d\tilde{r} d\tilde{z}. \quad (2.16)$$

The integral in the right hand side can be solved to

$$\int_0^1 \int_0^{1-\tilde{z}} \tilde{r}(\tilde{r}, \tilde{z}) \, d\tilde{r} d\tilde{z} = \frac{1}{6} \left\{ 3a_r + (b_r - a_r) + (c_r - a_r) \right\} \quad (2.17)$$

which reduces the whole equation to

$$\begin{aligned} \nabla f \cdot 2\pi \cdot \iint r \, dr dz &= \nabla f \cdot 2\pi \cdot |(b_r - a_r)(c_z - a_z) - (c_r - a_r)(b_z - a_z)| \\ &\quad \cdot \frac{1}{6} \left\{ 3a_r + (b_r - a_r) + (c_r - a_r) \right\}. \end{aligned} \quad (2.18)$$

Substituting

$$G = \left| (b_r - a_r)(c_z - a_z) - (c_r - a_r)(b_z - a_z) \right| \cdot \frac{1}{6} \left\{ 3a_r + (b_r - a_r) + (c_r - a_r) \right\} \quad (2.19)$$

one can write

$$\iiint \nabla f \cdot r \, dr d\theta dz = \nabla f \cdot 2\pi \cdot G. \quad (2.20)$$

2.3 Right hand side

For a polygonal mesh the right hand side of the equation above can be considered as a sum of line integrals

$$\oint_S f \cdot \vec{n} \, dS = \iint f(\vec{r}(t, s)) \cdot \underbrace{\frac{\frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s}}{\left\| \frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s} \right\|}}_{\vec{n}} \cdot \left\| \frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s} \right\| \, dt ds \quad (2.21)$$

which reduces to

$$\oint_S f \cdot \vec{n} \, dS = \iint f(\vec{r}(t, s)) \cdot \left(\frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s} \right) \, dt ds. \quad (2.22)$$

For the parametrization the choice is made

$$r = r(t) \quad (2.23)$$

$$\theta = s \quad (2.24)$$

$$z = z(t) \quad (2.25)$$

which leads to

$$\frac{\partial \vec{r}(t, s)}{\partial t} = \begin{pmatrix} \frac{\partial r(t)}{\partial t} \\ 0 \\ \frac{\partial z(t)}{\partial t} \end{pmatrix} \quad (2.26)$$

and

$$\frac{\partial \vec{r}(t, s)}{\partial s} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (2.27)$$

hence

$$\left(\frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s} \right) = \begin{pmatrix} -\frac{\partial z(t)}{\partial t} \\ 0 \\ \frac{\partial r(t)}{\partial t} \end{pmatrix} \quad (2.28)$$

and

$$\left\| \frac{\partial \vec{r}(t, s)}{\partial t} \times \frac{\partial \vec{r}(t, s)}{\partial s} \right\| = \sqrt{\frac{\partial r(t)}{\partial t}^2 + \frac{\partial z(t)}{\partial t}^2}. \quad (2.29)$$

2.3.1 Surface Integral

Assuming a surface integral for a polygonal cell

$$S = \int_0^{2\pi} \left[\sum_i \int_0^{l_i} r_i(t) \, dt \right] d\theta \quad (2.30)$$

with r_i independent of θ leads to

$$S = 2\pi \sum_i \int_0^{l_i} r_i(t) \, dt. \quad (2.31)$$

2.3.2 Function integral

The approach above can be extended with a function f and an normal vector

$$\oint_S f \cdot \vec{n} dS = \int_0^{2\pi} \left[\sum_i \vec{n}_i \int_0^{l_i} f_i(t) \cdot r_i(t) dt \right] d\theta \quad (2.32)$$

again assuming an Independence of θ

$$\oint_S f \cdot \vec{n} dS = 2\pi \sum_i \vec{n}_i \int_0^{l_i} f_i(t) \cdot r_i(t) dt \quad (2.33)$$

The radius function r_i can be expressed as

$$r_i(t) = \frac{t}{l_i}(r_{i,1} - r_{i,0}) + r_{i,0} \quad (2.34)$$

a similar approach can be done for the function value f_i

$$f_i(t) = \frac{t}{l_i}(f_{i,1} - f_{i,0}) + f_{i,0}. \quad (2.35)$$

Using the above the integral in the sum can be solved as

$$\int_0^{l_i} f_i(t) \cdot r_i(t) dt = f_{i,1} \cdot \frac{l_i}{6} \cdot (2r_{i,1} + r_{i,0}) + f_{i,0} \cdot \frac{l_i}{6} \cdot (r_{i,1} + 2r_{i,0}) \quad (2.36)$$

which leads to the final result

$$\oint_S f \cdot \vec{n} dS = 2\pi \sum_i \vec{n}_i \left\{ f_{i,1} \cdot \frac{l_i}{6} \cdot (2r_{i,1} + r_{i,0}) + f_{i,0} \cdot \frac{l_i}{6} \cdot (r_{i,1} + 2r_{i,0}) \right\} \quad (2.37)$$

which using $l_i = |\vec{x}_{i+1} - \vec{x}_i| = |\vec{x}_{i+1,i}|$ can be rewritten as

$$\oint_S f \cdot \vec{n} dS = 2\pi \sum_i^N \vec{n}_i \left\{ f_{i+1} \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (2r_{i+1} + r_i) + f_i \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (r_{i+1} + 2r_i) \right\}. \quad (2.38)$$

As the in integral must be closed the last value in the chain is automatically the first one hence the inner sum can be rewritten as

$$\vec{n}_1 \left\{ f_2 \cdot \frac{|\vec{x}_{2,1}|}{6} \cdot (2r_2 + r_1) + f_1 \cdot \frac{|\vec{x}_{2,1}|}{6} \cdot (r_2 + 2r_1) \right\} \quad (2.39)$$

$$\vec{n}_2 \left\{ f_{i+1} \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (2r_{i+1} + r_i) + f_i \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (r_{i+1} + 2r_i) \right\} \quad (2.40)$$

$$\vec{n}_3 \left\{ f_1 \cdot \frac{|\vec{x}_{1,3}|}{6} \cdot (2r_1 + r_3) + f_3 \cdot \frac{|\vec{x}_{1,3}|}{6} \cdot (r_1 + 2r_3) \right\} \quad (2.41)$$

which leads to the reformulation

$$f_i \left(\vec{n}_{i+1} \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (r_{i+1} + 2r_i) + \vec{n}_{i-1} \cdot \frac{|\vec{x}_{i,i-1}|}{6} \cdot (2r_i + r_{i-1}) \right). \quad (2.42)$$

Taking this result the surface integral can be cast in the form

$$\oint_S f \cdot \vec{n} dS = 2\pi \sum_i^N f_i \left(\vec{n}_{i+1} \cdot \frac{|\vec{x}_{i+1,i}|}{6} \cdot (r_{i+1} + 2r_i) + \vec{n}_{i-1} \cdot \frac{|\vec{x}_{i,i-1}|}{6} \cdot (2r_i + r_{i-1}) \right). \quad (2.43)$$

Since the term $\vec{n}_{i+1} \cdot |\vec{x}_{i+1,i}|$ is just the non normalized outward verctor of the surface element it can be cast in the form

$$\vec{n}_{i+1} \cdot |\vec{x}_{i+1,i}| = M \cdot \vec{x}_{i+1,i} \quad (2.44)$$

where M is a rotation matrix defined as

$$M = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.45)$$

which for $\theta = -\pi/2$ is

$$M = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (2.46)$$

hence

$$\begin{aligned} \oint_S f \cdot \vec{n} dS &= \frac{2}{6}\pi \sum_i^N f_i \left[M \cdot \vec{x}_{i+1,i} \cdot (r_{i+1} + 2r_i) + M \cdot \vec{x}_{i,i-1} \cdot (2r_i + r_{i-1}) \right] \\ &= \frac{2}{6}\pi M \cdot \sum_i^N f_i \left[\vec{x}_{i+1,i} \cdot (r_{i+1} + 2r_i) + \vec{x}_{i,i-1} \cdot (2r_i + r_{i-1}) \right]. \end{aligned} \quad (2.47)$$

2.4 Gradient - Triangular Mesh

For a triangular mesh the the gradient can be formulated as

$$\iiint \nabla f \cdot r dr d\theta dz = \oint_S f \cdot \vec{n} dS \quad (2.48)$$

$$\nabla f \cdot 2\pi \cdot G = \frac{2}{6}\pi M \cdot \sum_i^N f_i \left[\vec{x}_{i+1,i} \cdot (r_{i+1} + 2r_i) + \vec{x}_{i,i-1} \cdot (2r_i + r_{i-1}) \right] \quad (2.49)$$

which reduces to

$$\nabla f = \frac{M}{6G} \cdot \sum_{i=1}^3 f_i \left[\vec{x}_{i+1,i} \cdot (r_{i+1} + 2r_i) + \vec{x}_{i,i-1} \cdot (2r_i + r_{i-1}) \right]. \quad (2.50)$$

2.5 Laplace - Triangular Mesh

Using the divergence theorem in cylinder coordinates and assuming a triangular mesh, $\frac{\partial}{\partial \theta} = 0$ and $\nabla^2 f$ to be constant over the cell

$$\begin{aligned}
\int_V \nabla^2 f \, dV &= \oint_S \nabla f \cdot \vec{n} \, dS \\
\iiint \nabla^2 f \cdot r \, dr d\theta dz &= \int_0^{2\pi} \left[\sum_b \vec{n}_b \int_0^{l_b} \nabla f_b(t) \cdot r_b(t) \, dt \right] d\theta \\
2\pi \cdot \nabla^2 f_i \cdot \underbrace{\sum_{c=1}^N G_c}_{G_{tot}} &= \frac{2\pi}{6} M \cdot \sum_{b=1}^N \nabla f_b \left[\vec{x}_{b+1,b} \cdot (r_{b+1} + 2r_b) + \vec{x}_{b,b-1} \cdot (2r_b + r_{b-1}) \right] \\
\nabla^2 f_i &= \frac{M}{6 G_{tot}} \cdot \sum_{b=1}^N \nabla f_b \left[\vec{x}_{b+1,b} \cdot (r_{b+1} + 2r_b) + \vec{x}_{b,b-1} \cdot (2r_b + r_{b-1}) \right]
\end{aligned} \tag{2.51}$$

using the definition above

$$\begin{aligned}
\nabla^2 f_i &= \frac{M^2}{36 G_{tot}} \cdot \sum_{b=1}^N \frac{1}{G_b} \left\{ \right. \\
&\quad \left(\sum_{b_i=1}^3 f_{b_i} \left[\vec{x}_{b_i+1,b_i} \cdot (r_{b_i+1} + 2r_{b_i}) + \vec{x}_{b_i,b_i-1} \cdot (2r_{b_i} + r_{b_i-1}) \right] \right) \\
&\quad \cdot \left[\vec{x}_{b+1,b} \cdot (r_{b+1} + 2r_b) + \vec{x}_{b,b-1} \cdot (2r_b + r_{b-1}) \right] \left. \right\}.
\end{aligned} \tag{2.52}$$