Constitutive equations

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Cell Method for multiphysics problems

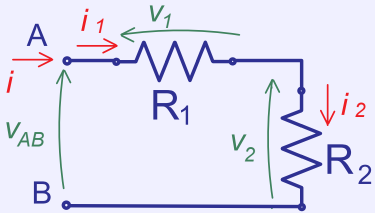
Outline

Equation classification

topological and constitutive equations

- As pointed out in the first lesson, two kinds of equations constraint global variables:
- topological equations which:
  - link together global variables of the same kind (source or configuration)
  - do not depend on metric
  - are exact on the given discretization
- constitutive equations which:
  - link together variables of different kind (one source with one configuration)
  - depend on metric and on material characteristics
  - are approximate

constraint equations



topological or Kirchhoff laws

$$i = i_1 = i_2 \qquad (1)$$
$$v_{AB} - v_1 - v_2 = 0 \qquad (2)$$

constitutive equations

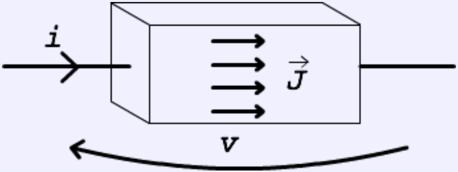
$$v_1 = R_1 i_1 \qquad (3)$$
$$v_2 = R_2 i_2 \qquad (4)$$

$$R_1 = \rho_1 \frac{l_1}{S_1}, \quad R_2 = \rho_2 \frac{l_2}{S_2} \qquad (5)$$

$$v_{AB} = v_1 + v_2 = R_1 i_1 + R_2 i_2 = (R_1 + R_2)\, i = R_{eq} i \qquad (6)$$

hypothesis on field variation

- constitutive equations link together the source variable current i flowing through the component to the configuration variable v across its terminals
- the second Ohm law used to compute the value of R_1 and R_2 has been obtained under the hypothesis of a rectilinear conductor with constant conductor cross section and uniform distribution of current density $\vec{J}$,



characteristics of constitutive equations

- the need to impose hypothesis on the space distribution of field variables derives from the definition of macroscopic material equation which is expressed in terms of field variables $\overrightarrow{E} = \rho \overrightarrow{J}$:
- the "regular" distribution of field variables in space integration is needed to link field and global variables

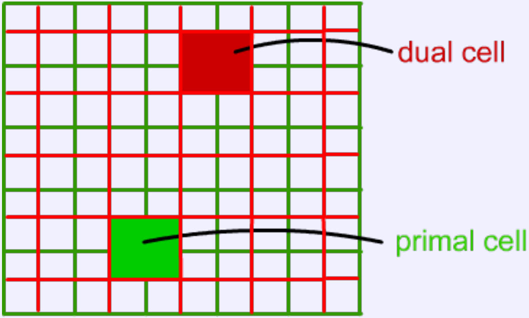
$$i = \int_S \overrightarrow{J} \cdot d\overrightarrow{S} = JS \Rightarrow J = \frac{i}{S} \tag{7}$$

$$v = \int_l \overrightarrow{E} \cdot d\overrightarrow{l} = El \Rightarrow E = \frac{v}{l} \tag{8}$$

$$\overrightarrow{E} = \rho \overrightarrow{J} \;\Rightarrow\; \frac{v}{l} = \rho \frac{i}{S} \;\Rightarrow\; v = \rho \frac{l}{S} i \tag{9}$$

two dimensional grids

- among possible ways of subdividing the problem geometry the orthogonal one is the simplest whenever it can be applied



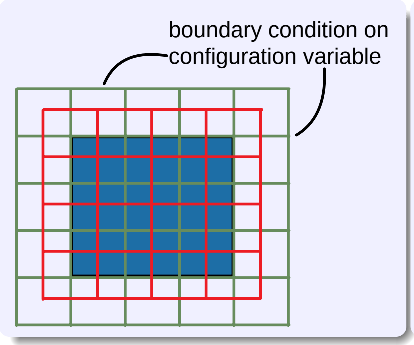
- in this case both primal and dual complex of cell are sharing the same "shape"

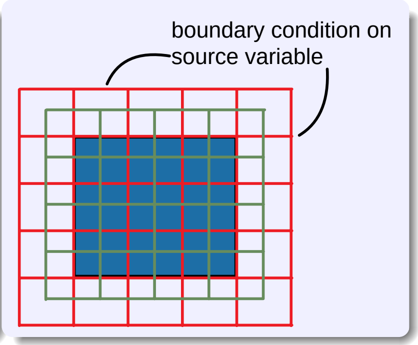
Primal or dual mesh?

solution variable

- Global variables are associated to primal or dual space elements
- the choice of the variable used in the solution influences the meaning of the discretization
  - magnetic flux $\leftrightarrow$ primal face
  - electric current $\leftrightarrow$ dual face
- since the shape of the cells is "regular" both in primal or dual complex, the choice of which grid defines the geometry (for instance following material interfaces) is just a matter of which variable is used for solution of the problem

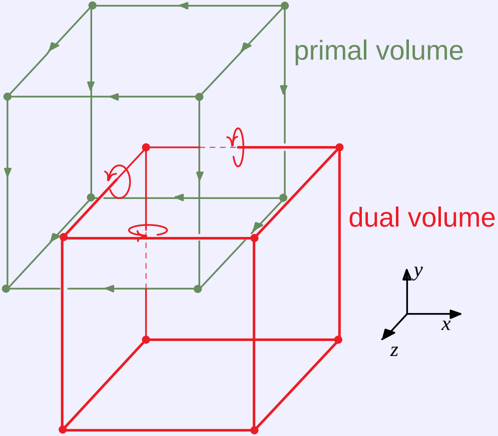
Primal or dual mesh?





three dimensional grids

- the same property holds also on three dimensional grids



variables linked by duality

- constitutive equations link global variables on a couple of dual geometrical entities
- two situations are possible:
  - primal face $\leftrightarrow$ dual edge
  - primal edge $\leftrightarrow$ dual face
- usually primal cell complex define geometry so that, even if geometrically similar, the two relations are treated in different ways

Constitutive matrix

$\Phi[\bar{S}] \longleftrightarrow F[\tilde{L}]$

$$\mathbf{B} = \mu_0 \mathbf{H} + \mu_0 \mathbf{M} \tag{10}$$

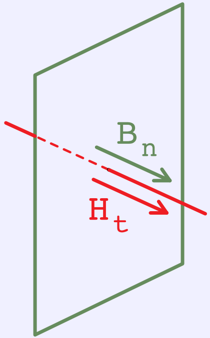
$$B_n = \frac{\Phi[\bar{S}]}{S} \tag{11}$$

$$H_t = \frac{F[\tilde{L}]}{L}$$

$$F_M[\tilde{L}] = \mathbf{M} \cdot \mathbf{L}$$

$$F = \frac{L}{\mu_0 S}\Phi[\bar{S}] - F_M \tag{12}$$

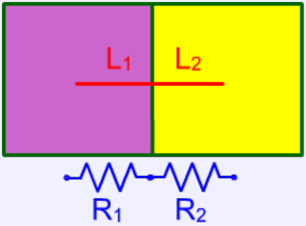
hypothesis: local uniformity of field variables and homogeneity of material



material inhomogeneity

- if the primal face falls on the interface between two materials with different properties, the additivity property of line integral $\int_L \mathbf{H} \cdot d\mathbf{l}$ is used to treat the constitutive equation as the series of two components, each one with its properties

$$R = \frac{L_1}{\mu_1 S} + \frac{L_2}{\mu_2 S} \tag{13}$$



Constitutive matrix

$u \longleftrightarrow i$

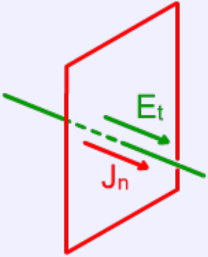
$$\mathbf{E} = \rho \mathbf{J} \tag{14}$$

$$E_t = \frac{u}{L} \tag{15}$$

$$J_n = \frac{i}{S}$$

$$u = \rho \frac{L}{S} i \tag{16}$$

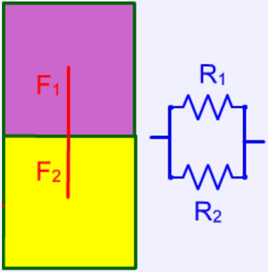
hypothesis: local uniformity of field variables and homogeneity of material



material inhomogeneity

- if the primal edge falls on the interface between two materials with different properties, the constitutive relation is treated as the parallel of two components, each one with its properties

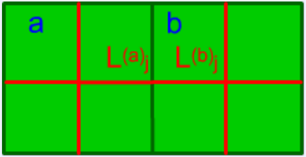
$$R = \left(\frac{F_1}{\rho_1 L} + \frac{F_2}{\rho_2 L} \right)^{-1} \tag{17}$$



building constitutive matrix

- as mentioned before, additivity property can be used to build constitutive equations breaking the dual edge or the dual face into two parts belonging to each primal cell

$$L_j = L_j^a \cup L_j^b \tag{18}$$



flowchart of cell by cell scheme

for i on all volumes

  build local interpolation with local orientation

  build local matrix $M^{(loc)}$

  for j on all entities in the volume

    store local matrix $M^{(loc)}$ in global one taking into account true orientation of elements

  end

end

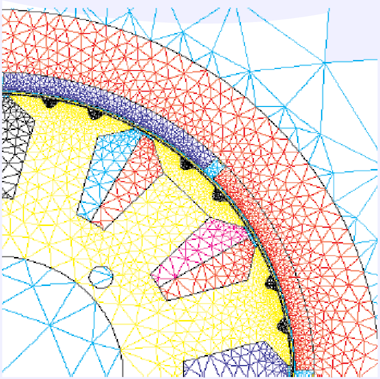
Why unstructured meshes?

square and circles

Why unstructured meshes?

Technical problems

- complex shapes
- uneven material boundaries
- objects of different dimensions in the same problem

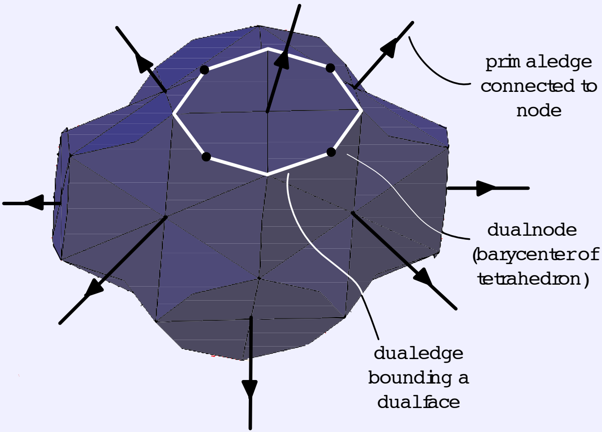


Barycentric complex

how to build a mesh dual to symplex

- one possible way to build a mesh dual to a symplectic one is to use barycentric mesh:
  - dual node $\leftarrow$ barycenter of symplex cell
  - dual edge $\leftarrow$ broken line joining two dual nodes and passing through the barycenter of the face which divides them
  - dual face $\leftarrow$ union of quadrilateral faces having as vertices: mid point of primal edge, barycenter of one face hinged on edge, barycenter of symplex cell, barycenter of the other face hinged on edge
  - dual volume $\leftarrow$ union of all volumes having dual faces as boundaries

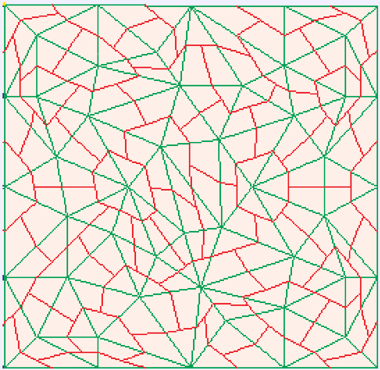
dual entities



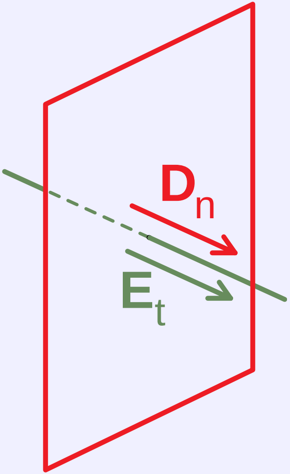
Primal or dual mesh?

simplex or polytope

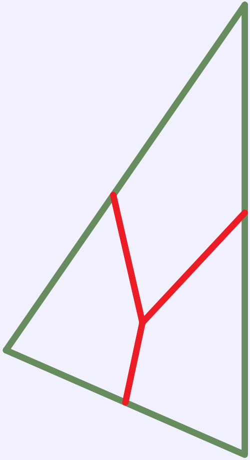
- quadrilateral orthogonal meshes share the same cell shape for primal or dual complex
- simplex mesh gives rise to a polygonal dual cell complex not suited for technical geometries
- solution variable must reside on simplex mesh



orthogonal



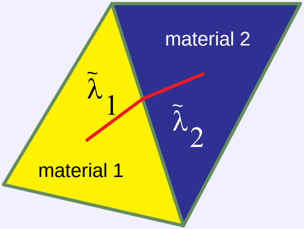
simplex



interpolation

1. from global variables get a local interpolation of fields inside cell
2. integrate field values over geometrical entities
3. assembly global variables

$$F = \int_{\tilde{\lambda}_1} \mathbf{H} \cdot d\mathbf{l} + \int_{\tilde{\lambda}_2} \mathbf{H} \cdot d\mathbf{l} \quad (19)$$



Uniformity of field variables

hypothesis

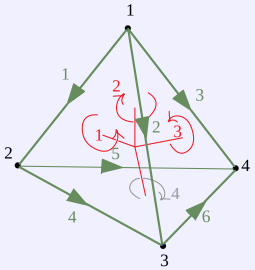
- the simplest way to build a local interpolation of field variables is to consider them uniform inside the cell
- this hypothesis is not always congruent with the regime of fields variation
- two constitutive relations are considered:
  - magnetic flux ϕ on primal faces $\leftrightarrow$ magneto-motive force F on dual edges
  - electric voltage u on primal edges $\leftrightarrow$ electric current/dielectric flux on dual faces

Gauss law for magnetic flux

$$\Phi_1 + \Phi_2 + \Phi_3 + \Phi_4 = 0 \quad (20)$$

$$\Phi_4 = -\Phi_1 - \Phi_2 - \Phi_3 \quad (21)$$

a uniform $\mathbf{B} = (B_x, B_y, B_z)$ is consistent with flux solenoidality



Uniformity of field variables

area vector **S**

$$\mathbf{S}_i = A_i \mathbf{n}_i \quad (22)$$

$$\Phi_i = \mathbf{B} \cdot \mathbf{S}_i = B_x S_{ix} + B_y S_{iy} + B_z S_{iz} \quad (23)$$

$$\{\Phi'\} = \left\{ \begin{array}{c} \Phi_1 \\ \Phi_2 \\ \Phi_3 \end{array} \right\} \quad (24)$$

$$\{B\} = \left\{ \begin{array}{c} B_x \\ B_y \\ B_z \end{array} \right\} \quad (25)$$

$$\{\Phi'\} = [S]\,\{B\} \quad (26)$$

$$\{B\} = [S]^{-1}\,\{\Phi'\} \quad (27)$$

Uniformity of field variables

from square (3×3) matrix $[S]^{-1}$ a rectangular (3×4) one can be obtained by inserting a column of zeros in Φ_4 position so that

$$[S]^{-1} = \begin{bmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{bmatrix} \tag{28}$$

$$[S^a]^{-1} = \begin{bmatrix} m_{11} & m_{12} & m_{13} & 0 \\ m_{21} & m_{22} & m_{23} & 0 \\ m_{31} & m_{32} & m_{33} & 0 \end{bmatrix} \tag{29}$$

Uniformity of field variables

$$\{B\} = [S^a]^{-1} \{\Phi\} \tag{30}$$

$$\mathbf{H} = \nu \mathbf{B} \tag{31}$$

$$\tilde{L}_i = (\tilde{L}_{ix}, \tilde{L}_{iy}, \tilde{L}_{iz}) \tag{32}$$

$$F_i = \tilde{L}_i \cdot \mathbf{H} \tag{33}$$

$$\{F\} = \left[\tilde{L}\right] \nu \, [S^a]^{-1} \{\Phi\} = \left[M_\nu^{(loc)}\right] \{\Phi\} \tag{34}$$

irrotational **E**

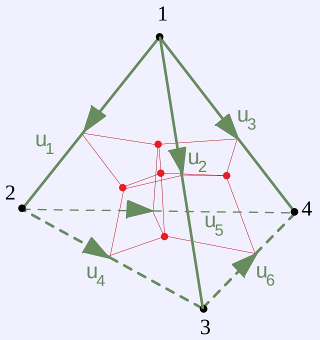
in static conditions $\mathbf{E} = -\nabla\phi$

$$u_1 - u_2 + u_4 = 0 \tag{35}$$

$$u_4 = -u_1 + u_2 \tag{36}$$

only 3 out of 6 u values are independent

a uniform $\mathbf{E} = (E_x, E_y, E_z)$ is consistent with electric field irrotationality



Uniformity of field variables

edge vector **L**

$$u_i = \mathbf{E} \cdot \mathbf{L}_i = E_x L_{ix} + E_y L_{iy} + E_z L_{iz} \quad (37)$$

$$\{u'\} = \begin{Bmatrix} u_1 \\ u_2 \\ u_3 \end{Bmatrix} \quad (38)$$

$$\{E\} = \begin{Bmatrix} E_x \\ E_y \\ E_z \end{Bmatrix} \quad (39)$$

$$\{u'\} = [L]\{E\} \quad (40)$$

$$\{E\} = [L]^{-1}\{u'\} \quad (41)$$

Uniformity of field variables

from square (3×3) matrix $[L]^{-1}$ a rectangular (3×6) one can be obtained by inserting three columns of zeros in u_4, u_5, u_6 positions so that

$$\{E\} = [L^a]^{-1} \{u\} \tag{42}$$

$$\mathbf{D} = \epsilon \mathbf{E} \tag{43}$$

$$\tilde{S}_i = (\tilde{S}_{ix}, \tilde{S}_{iy}, \tilde{S}_{iz}) \tag{44}$$

$$\Psi_i = \tilde{S}_i \cdot \mathbf{D} \tag{45}$$

$$\{\Psi\} = \left[\tilde{S}\right] \epsilon [L^a]^{-1} \{u\} = \left[M_\epsilon^{(loc)}\right] \{u\} \tag{46}$$

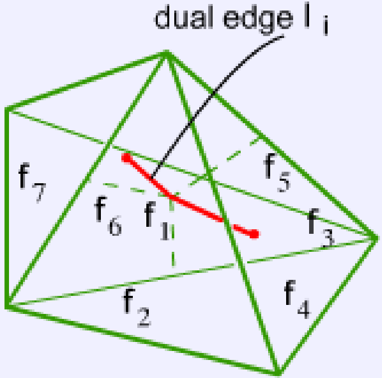
Remarks

- local interpolation involves almost all global variables defined over the cell (ϕ_1, ϕ_2, ϕ_3) or (u_1, u_2, u_3)
- local matrices containing geometrical quantities ($[S]^{-1}$, $[L]^{-1}$) are full matrices
- resulting local matrices $\left[M_\nu^{(loc)}\right]$ and $\left[M_\epsilon^{(loc)}\right]$ are full matrices linking global variables defined over the cell
- global constitutive matrix is not anymore diagonal, like in orthogonal meshes, but has a sparse structure

sparsity pattern

non-null elements in first row of matrix $[M_\nu]$

$M_{\nu 11}, M_{\nu 12}, M_{\nu 13}, M_{\nu 14}, M_{\nu 15}, M_{\nu 16}, M_{\nu 17}$



field regimes

- solenoidality of magnetic flux holds in any case
- irrotationality of electric field holds only in static conditions when electromagnetic induction is not present

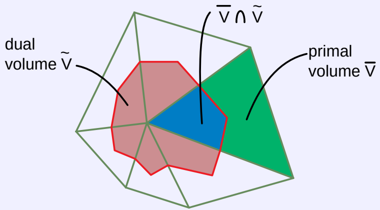
$$\oint \mathbf{E} \cdot d\mathbf{l} = -\frac{d\phi}{dt} \qquad (47)$$

- in this case all six values of u are independent and uniform **E** hypothesis does not hold anymore
- affine law of variation of field variable **E** can be implemented in different ways
  - micro-cell approach
  - Whitney shape function approach

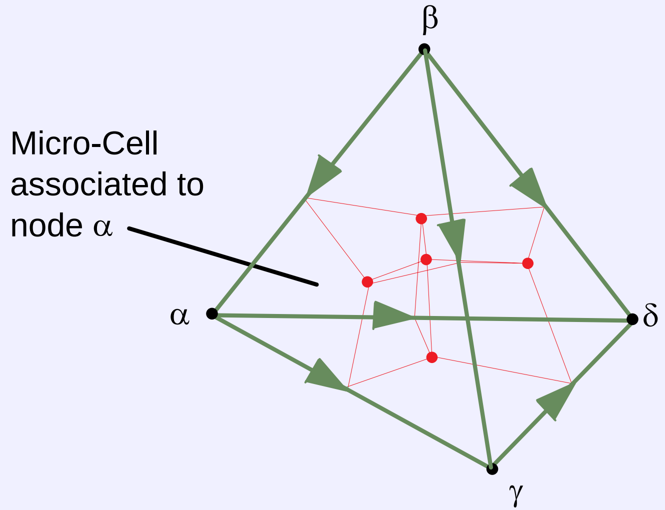
Micro-cell approach

rationale

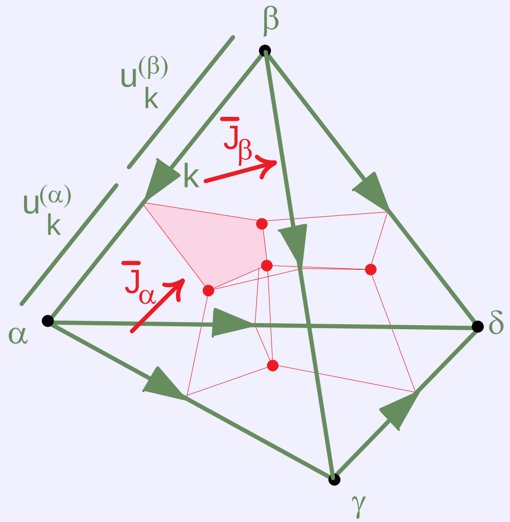
- micro-cell approach implements a computational scheme similar to that of uniform field but field uniformity is considered valid only on a portion of the cell
- additivity of integral quantities is used to link local fields to global variables



Micro-cell approach



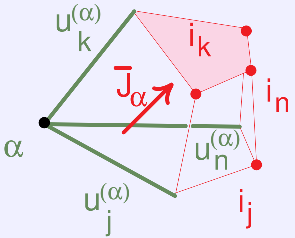
Micro-cell approach



Micro-cell approach

$$\left\{ \begin{array}{c} i_k \\ i_j \\ i_n \end{array} \right\} = \left[\begin{array}{ccc} \tilde{S}_{kx} & \tilde{S}_{ky} & \tilde{S}_{kz} \\ \tilde{S}_{jx} & \tilde{S}_{jy} & \tilde{S}_{jz} \\ \tilde{S}_{nx} & \tilde{S}_{ny} & \tilde{S}_{nz} \end{array} \right] \left\{ \begin{array}{c} J_x^{(\alpha)} \\ J_y^{(\alpha)} \\ J_z^{(\alpha)} \end{array} \right\} \quad (48)$$

$$\{i^{(\alpha)}\} = \left[\tilde{S}_\alpha\right] \mathbf{J}^{(\alpha)} \quad (49)$$



Micro-cell approach

electro-motive force

$$\left\{ \begin{array}{c} J_x^{(\alpha)} \\ J_y^{(\alpha)} \\ J_z^{(\alpha)} \end{array} \right\} = \left[\tilde{S}_\alpha\right]^{-1} \left\{ \begin{array}{c} i_k \\ i_j \\ i_n \end{array} \right\} \quad (50)$$

$$\{u^{(\alpha)}\} = [L_\alpha]\,\rho\left[\tilde{S}_\alpha\right]^{-1}\{i^{(\alpha)}\} \quad (51)$$

$$u_k = u_k^{(\alpha)} + u_k^{(\beta)} = \rho\left([L_\alpha]\left[\tilde{S}_\alpha\right]^{-1}\{i^{(\alpha)}\} + [L_\beta]\left[\tilde{S}_\beta\right]^{-1}\{i^{(\beta)}\}\right) \quad (52)$$

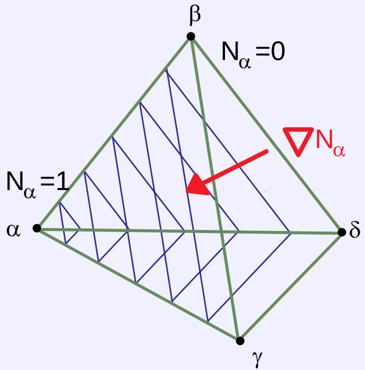
Whitney interpolation approach

rationale

- Whitney shape function have been widely used in finite elements to interpolate vector quantities
- they can also be used here to interpolate field inside tetrahedra starting from global quantities on edges or faces
- Whitney shape functions enforce inter-element continuity of field components (normal component of flux density or tangential component of electric field)
- the use of Whitney shape functions gives rise to solution matrices which are identical to the ones of vector based finite elements

nodal shape functions

$$N_\alpha = a_\alpha x + b_\alpha y + c_\alpha z + d_\alpha \quad (53)$$



geometrical interpretation of gradient vector

- the gradient vector can be related to tetrahedron volume

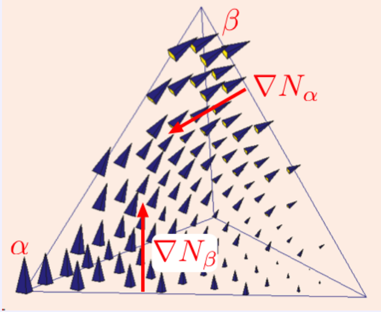
$$Volume = \frac{1}{3} h_1 F_1 \quad \Rightarrow \quad h_1 F_1 = 3 * Volume \tag{54}$$

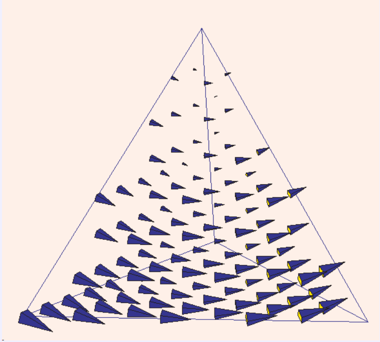
- ∇N_1 vector is orthogonal to face opposite to node 1 and makes the function goes from value 0 to 1 along the perpendicular direction so that:

$$\nabla N_1 = \frac{1}{h_1} \frac{\overrightarrow{F_1}}{|\overrightarrow{F_1}|} = \frac{\overrightarrow{F_1}}{3 * Volume} \tag{55}$$

vector shape functions

$$\bar{w}_k = N_\alpha \nabla N_\beta - N_\beta \nabla N_\alpha \quad (56)$$





vector shape functions

$$u_k = \int_{L_k} \bar{E} \cdot d\bar{l} \tag{57}$$

$$\bar{E}(P) = \sum_{k=1}^{6} u_k \bar{w}_k \tag{58}$$

$$i_n = \int_{\tilde{S}_n} \bar{J} \cdot d\bar{S} = \int_{\tilde{S}_n} \sigma \sum_{k=1}^{6} u_k \bar{w}_k \cdot d\bar{S} = \tag{59}$$

$$= \sum_{k=1}^{6} \sigma u_k \int_{\tilde{S}_n} \bar{w}_k \cdot d\bar{S} = \sum_{k=1}^{6} c_{nk} u_k$$

Comparison

equilateral tetrahedron

Micro-cell

$$\begin{bmatrix} 1.000 & -0.80E-04 & 0.10E-03 & 0.80E-04 & -0.10E-03 & 0.76E-08 \\ -0.80E-04 & 1.000 & 0.10E-03 & -0.80E-04 & 0.76E-08 & -0.10E-03 \\ -0.44E-04 & -0.44E-04 & 1.000 & 0.11E-19 & -0.44E-04 & -0.44E-04 \\ 0.0000 & 0.0000 & 0.0000 & 1.000 & 0.0000 & 0.0000 \\ -0.15E-03 & 0.24E-07 & -0.15E-03 & 0.35E-04 & 1.000 & -0.35E-04 \\ 0.24E-07 & -0.15E-03- & 0.15E-03- & 0.35E-04 & -0.35E-04 & 1.000 \end{bmatrix}$$

Whitney

$$\begin{bmatrix} 1.0000 & 0.1667 & 0.1666 & 0.1667 & 0.1667 & 0.36E-04 \\ 0.1667 & 1.000 & 0.1666 & -0.1667 & 0.36E-04 & 0.1667 \\ 0.1666 & 0.1666 & 1.000 & 0.15E-16 & -0.1666 & -0.1666 \\ 0.1667 & -0.1667 & 0.51E-17 & 1.000 & 0.1667 & -0.1667 \\ 0.1667 & 0.36E-04 & -0.1666 & 0.1667 & 1.000 & 0.1667 \\ 0.36E-04 & 0.1667 & -0.1666 & -0.1667 & 0.1667 & 1.000 \end{bmatrix}$$

power on primal cell

- power dissipated in one volume can be expressed as:

$$P = \int_\Omega \vec{E} \cdot \vec{J} \, d\Omega \tag{60}$$

- by interpolating electric field by means of Whitney edge functions

$$\vec{E} = \sum_{k=1}^{6} u_k \bar{w}_k \Rightarrow P = \int_\Omega \sum_{k=1}^{6} u_k \vec{w}_k \cdot \vec{J} \, d\Omega \tag{61}$$

- by considering that $\vec{J}$ would be uniform on Ω

$$P = \sum_{k=1}^{6} u_k \vec{J} \cdot \int_\Omega \vec{w}_k d\Omega \tag{62}$$

power on primal cell

- due to the geometrical property of the Whitney edge function, the following relation holds:

$$\tilde{S}_k = \int_\Omega \vec{w}_k d\Omega \tag{63}$$

- the previous equation becomes:

$$P = \sum_{k=1}^{6} u_k \vec{J} \cdot \tilde{S}_k = i_k \tag{64}$$

- so that power can be written as:

$$P = \sum_{k=1}^{6} u_k i_k \tag{65}$$

power on primal cell

- $$P = \sum_{k=1}^{6} u_k i_k \quad (66)$$
- going back to the first definition of power P

$$P = \int_{\Omega} \vec{E} \cdot \vec{J} d\Omega = \sum_{k=1}^{6} u_k \underbrace{\int_{\Omega} \vec{w}_k \cdot \sigma \sum_{n=1}^{6} \vec{w}_n u_n d\Omega} \quad (67)$$

- by comparing the two equations, the term underbraced is equal to i_k

power on primal cell

- k-th current tailored to cell Ω is thus written as:

$$i_k = \sum_{n=1}^{6} u_n \int_{\Omega} \vec{w}_k \cdot \sigma \vec{w}_n d\Omega \qquad (68)$$

- by expressing the terms of the previous equation as matrix element:

$$i_k = \sum_{n=1}^{6} M_{kn} u_n \qquad (69)$$

where

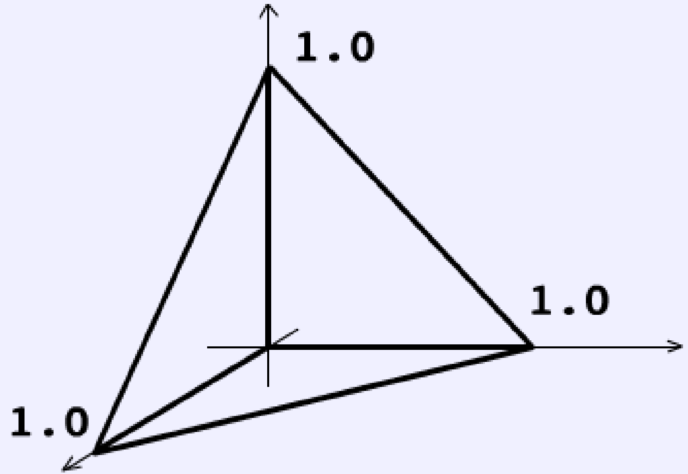
$$M_{kn} = \sigma \int_{\Omega} \vec{w}_k \cdot \vec{w}_n d\Omega \qquad (70)$$

symmetric constitutive matrix

constitutive matrix

- the constitutive matrix obtained has a symmetric structure and it is often referred to as Galerkin matrix since it is formally equal to the one obtained by weighted residual (Galerkin) finite element matrix if edge vector shape functions are used
- symmetry of the matrix allows to state some mathematical properties of the resulting system of equations ensuring its stability when time-marching scheme are used

example on orthogonal tetrahedron



example on orthogonal tetrahedron

Whitney

1.0000e+00	4.4118e-01	4.4118e-01	2.9412e-02	2.9412e-02	0
4.4118e-01	1.0000e+00	4.4118e-01	-2.9412e-02	0	2.9412e-02
4.4118e-01	4.4118e-01	1.0000e+00	0	-2.9412e-02	-2.9412e-02
-6.8627e-02	6.8627e-02	0	3.3333e-01	6.8627e-02	-6.8627e-02
-6.8627e-02	0	6.8627e-02	6.8627e-02	3.3333e-01	6.8627e-02
0	-6.8627e-02	6.8627e-02	-6.8627e-02	6.8627e-02	3.3333e-01

Whitney symmetric

1.0000e+00	5.0000e-01	5.0000e-01	4.6317e-16	4.5797e-16	0
5.0000e-01	1.0000e+00	5.0000e-01	-4.6317e-16	0	4.7184e-16
5.0000e-01	5.0000e-01	1.0000e+00	0	-4.5797e-16	-4.5797e-16
4.6317e-16	-4.6317e-16	0	4.0000e-01	1.0000e-01	-1.0000e-01
4.5797e-16	0	-4.5797e-16	1.0000e-01	4.0000e-01	1.0000e-01
0	4.7184e-16	-4.5797e-16	-1.0000e-01	1.0000e-01	4.0000e-01