

Vector Analysis in Orthogonal Curvilinear Coordinate System

A symbolic approch

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Summary

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Motivations

- In plasma physics research, vector analysis is ubiquitous but often tedious, and the cumbersomeness has even become a trait of the field.
- The automatic symbolic derivation is necessary (at least for me).
- Two symbolic approaches towards the vector analysis in general coordinate systems have been developed.
 - GVA [1] (General Vector Analysis), by Prof. Qin in 1997, a *Mathematica* package. Non-normalized basis is used, which has great generality and theoretical conciseness in any well-defined coordinates. However, we prefer to normalize the basis vectors in orthogonal curvilinear coordinates as is commonly shown in textbooks and cheatsheets.
 - SymFields [2], by Dr. Chu in 2020, a python package. It is also developed for vector analysis in the general coordinates. The package normalize basis vectors in both orthogonal and non-orthogonal coordinates, which complicates the mathematics and brings inconvenience for further developments (e.g. add more supports about 2-rank tensor related calculation).

Basic rules

- The metric tensor completely determines the geometric structure of the space [3].
- We usually use Einstein summation convention in the suffix notation [4, 5], a free suffix represents a equation and the summation always has one suffix up and another down (one contravariant and another covariant).
- The matric tensor \vec{G} and its coefficients q_{ik} and q^{ik}

$$\vec{G} = g_{ik}\vec{e}^{i}\vec{e}^{k} = g^{ik}\vec{e}_{i}\vec{e}_{k}$$

$$g_{ik} = \vec{e}_{i} \cdot \vec{e}_{k} = g_{ki}$$

$$g^{ik} = \vec{e}^{i} \cdot \vec{e}^{k} = g^{ki}$$

$$g_{ik} = \frac{\partial x}{\partial x^{i}}\frac{\partial x}{\partial x^{k}} + \frac{\partial y}{\partial x^{i}}\frac{\partial y}{\partial x^{k}} + \frac{\partial z}{\partial x^{i}}\frac{\partial z}{\partial x^{k}}$$

$$g^{ik} = \frac{\partial x^{i}}{\partial x}\frac{\partial x^{k}}{\partial x} + \frac{\partial x^{i}}{\partial y}\frac{\partial x^{k}}{\partial y} + \frac{\partial x^{i}}{\partial z}\frac{\partial x^{k}}{\partial z}$$

$$(1)$$

The vector notation

$$\vec{v} = v^{i}\vec{e}_{i} = v_{i}\vec{e}^{i}$$

$$v^{i} = \vec{v} \cdot \vec{e}^{i} = g^{ik}v_{k} \quad v_{i} = \vec{v} \cdot \vec{e}_{i} = g_{ik}v^{k}$$

$$\vec{e}_{i} = g_{ik}\vec{e}^{k} \quad \vec{e}^{k} = g^{ik}\vec{e}_{i}$$

$$\vec{e}_{i} = \frac{\partial}{\partial \xi^{i}} = \frac{\partial}{\partial x}\frac{\partial x}{\partial \xi^{i}} + \frac{\partial}{\partial y}\frac{\partial y}{\partial \xi^{i}} + \frac{\partial}{\partial z}\frac{\partial z}{\partial \xi^{i}} = \hat{x}_{a}\frac{\partial x^{a}}{\partial \xi^{i}} = \frac{\partial \vec{R}}{\partial \xi^{i}}$$

$$\vec{e}^{i} = \nabla \xi^{i} = \frac{\partial \xi^{i}}{\partial x}\vec{e}_{x} + \frac{\partial \xi^{i}}{\partial y}\vec{e}_{y} + \frac{\partial \xi^{i}}{\partial z}\vec{e}_{z}$$

$$\vec{e}^{1} = \frac{1}{V}(\vec{e}_{2} \times \vec{e}_{3}), \quad \vec{e}^{2} = \frac{1}{V}(\vec{e}_{3} \times \vec{e}_{1}), \quad \vec{e}^{3} = \frac{1}{V}(\vec{e}_{1} \times \vec{e}_{2})$$

$$\vec{e}_{1} = V(\vec{e}^{2} \times \vec{e}^{3}), \quad \vec{e}_{2} = V(\vec{e}^{3} \times \vec{e}^{1}), \quad \vec{e}_{3} = V(\vec{e}^{1} \times \vec{e}^{2})$$

$$\delta^{i}_{i} = \vec{e}^{i} \cdot \vec{e}_{i}$$

■ The Jacobian \mathcal{J} or V (volume of the space spaned by 3 covariant basis vectors)

$$\mathcal{J} = \frac{\partial(x, y, z)}{\partial(x^{1}, x^{2}, x^{3})} = \begin{vmatrix} \frac{\partial x}{\partial x^{1}} & \frac{\partial x}{\partial x^{2}} & \frac{\partial x}{\partial x^{3}} \\ \frac{\partial y}{\partial x^{1}} & \frac{\partial y}{\partial x^{2}} & \frac{\partial y}{\partial x^{3}} \\ \frac{\partial z}{\partial x^{1}} & \frac{\partial z}{\partial x^{2}} & \frac{\partial z}{\partial x^{3}} \end{vmatrix}$$

$$\mathcal{J}^{-1} = \frac{\partial(x^{1}, x^{2}, x^{3})}{\partial(x, y, z)} = \begin{vmatrix} \frac{\partial x^{1}}{\partial x} & \frac{\partial x^{1}}{\partial x} & \frac{\partial x^{1}}{\partial z} \\ \frac{\partial x^{2}}{\partial x} & \frac{\partial x^{2}}{\partial y} & \frac{\partial x^{2}}{\partial z} \\ \frac{\partial x^{3}}{\partial x} & \frac{\partial x^{3}}{\partial y} & \frac{\partial x^{3}}{\partial z} \end{vmatrix}$$

$$\mathcal{J} = V = \sqrt{\det |g_{ij}|} = \sqrt{g} = \vec{e}_{1} \cdot \vec{e}_{2} \times \vec{e}_{3}$$

$$\mathcal{J}^{-1} = \frac{1}{V} = \frac{1}{\sqrt{\det |g_{ij}|}} = \frac{1}{\sqrt{g}} = \vec{e}^{1} \cdot \vec{e}^{2} \times \vec{e}^{3}$$

$$g = \det |g_{ij}| = \mathcal{J}^{2} = V^{2} = \frac{g_{22}g_{33} - g_{23}^{2}}{g^{11}} = \frac{g_{11}g_{33} - g_{13}^{2}}{g^{22}} = \frac{g_{11}g_{22} - g_{12}^{2}}{g^{33}}$$
(3)

Differentiation of basis vectors

$$\nabla \cdot \vec{e}_i = \frac{1}{V} \frac{\partial V}{\partial x^i} = \frac{1}{2g} \frac{\partial g}{\partial x^i}, \quad (i = 1, 2, 3)$$

 $\nabla \times \vec{e}^i = 0$

$$(\vec{e}_{\sigma} \cdot \nabla) \, \vec{e}_{\rho} = \frac{1}{2} g^{\mu \lambda} \left(\frac{\partial g_{\rho \lambda}}{\partial x^{\sigma}} + \frac{\partial g_{\sigma \lambda}}{\partial x^{\rho}} - \frac{\partial g_{\rho \sigma}}{\partial x^{\lambda}} \right) \vec{e}_{\mu} = \Gamma^{\mu}_{\rho \sigma} \vec{e}_{\mu}, \quad (\rho, \sigma = 1, 2, 3)$$
(4)

The Christoffel symbol of the first kind is the *j*th covariant component of the vector $\partial \vec{e}_i/\partial x^k$

$$\Gamma_{jik} = \vec{e}_j \cdot \frac{\partial \vec{e}_i}{\partial x^k} = \frac{1}{2} \left(\frac{\partial g_{ji}}{\partial x^k} + \frac{\partial g_{jk}}{\partial x^i} - \frac{\partial g_{ik}}{\partial x^j} \right) \tag{5}$$

The Christoffel symbol of the second kind is the jth contravariant component of the vector $\partial \vec{e}_i/\partial x^k$

$$\Gamma^{j}_{ik} = \vec{e}_{j} \cdot \frac{\partial \vec{e}_{i}}{\partial x^{k}} = \frac{1}{2} g^{jn} \left(\frac{\partial g_{ni}}{\partial x^{k}} + \frac{\partial g_{nk}}{\partial x^{i}} - \frac{\partial g_{ik}}{\partial x^{n}} \right)$$
(6)

 $\Gamma_{jik}=\Gamma_{jki},\quad \Gamma_{jk}^j=\Gamma_{ki}^j,\quad \Gamma_{jik}=g_{jn}\Gamma_{ik}^n,\quad \Gamma_{jk}^j=g^{jn}\Gamma_{nik}$ Y. Ma • Vector Analysis in Orthogonal Curvilinear Coordinate System • April 4, 2023

Dot, cross

$$\vec{a} \cdot \vec{b} = a^{i}b_{i} = a_{i}b^{i} = g_{ij}a^{i}b^{j} = g^{ij}a_{i}b_{j}$$

$$\vec{a} \times \vec{b} = \epsilon^{ijk}Va^{i}b^{j}\vec{e}^{k} = \epsilon_{ijk}\frac{1}{V}a_{i}b_{j}\vec{e}_{k}$$
(7)

Gradient

$$\nabla = \vec{e}^{i} \frac{\partial}{\partial x^{i}}$$

$$\nabla \phi = \frac{\partial \phi}{\partial x^{i}} \vec{e}^{i}$$

$$\nabla \vec{f} = f_{\rho;\sigma} \vec{e}^{\sigma} \vec{e}^{\rho}$$

$$f_{\rho;\sigma} = \vec{e}_{\rho} \vec{e}_{\sigma} : \nabla \vec{f} = \frac{\partial f_{\rho}}{\partial x^{\sigma}} - \Gamma^{\mu}_{\rho\sigma} f_{\mu}$$

$$\nabla \nabla \vec{f} = f_{\rho;\sigma;\mu} \vec{e}^{\mu} \vec{e}^{\sigma} \vec{e}^{\rho}$$

$$f_{\rho;\sigma;\mu} = \frac{\partial f_{\rho;\sigma}}{\partial x^{\mu}} - \Gamma^{\lambda}_{\rho\mu} f_{\lambda;\sigma} - \Gamma^{\lambda}_{\sigma\mu} f_{\rho;\lambda}$$

$$\vec{a} \cdot \nabla \vec{b} = \left(a^{i} \frac{\partial b^{i}}{\partial x^{i}} + a^{i} b^{k} \Gamma^{j}_{ki} \right) \vec{e}_{k}$$
(8)

Divergence

$$\nabla \cdot \vec{f} = \nabla \cdot \left(f^{i} \vec{e}_{i} \right) = \vec{e}_{i} \cdot \nabla f^{i} + f^{i} \nabla \cdot \vec{e}_{i} = \frac{\partial f^{i}}{\partial x^{i}} + \frac{f^{i}}{2g} \frac{\partial g}{\partial x^{i}} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^{i}} \left(\sqrt{g} f^{i} \right)$$
(9)

$$\nabla \times \vec{f} = \frac{1}{\sqrt{g}} \frac{\partial f_i}{\partial x^j} \varepsilon_{kji} \vec{e}_k$$

$$\nabla \times \vec{f} = \frac{1}{\sqrt{g}} \left\{ \left(\frac{\partial f_3}{\partial x^2} - \frac{\partial f_2}{\partial x^3} \right) \vec{e}_1 + \left(\frac{\partial f_1}{\partial x^3} - \frac{\partial f_3}{\partial x^1} \right) \vec{e}_2 + \left(\frac{\partial f_2}{\partial x^1} - \frac{\partial f_1}{\partial x^2} \right) \vec{e}_3 \right\}$$
(10)

Differential of position vector

$$d\vec{r} = \frac{\partial \vec{r}}{\partial x^{i}} dx^{i} = dx^{i} \vec{e}_{i}$$

$$d\vec{r} = dx_{k} \vec{e}^{k} = g_{ik} dx^{i} \vec{e}^{k}$$

$$dx_{k} = g_{ik} dx^{i} \quad dx^{i} = g^{ik} dx_{k}$$

$$dx^{i} = \vec{e}^{i} \cdot d\vec{r} = \vec{e}^{i} \cdot \vec{e}_{i} dx^{j}$$

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Summary

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Python approach

Python can do symbolic calculations using the package sympy [6].

- Open source.
- Can run in the jupyter notebook interactively, which supports multiple output forms.
- Symbolic calculation ability cannot surpass that of Mathematica due to the procedural programming nature of the Python.

The software package OVA (Orthogonal curvilinear coordinate Vector Analysis) of Python version has been developed.

- OVA supports vector analysis in any well-defined right-handed orthogonal coordinate system.
- The 'Cartesian', 'Cylindrical' and 'Spherical' coordinates are built into OVA. The user can define a new coordinate system easily by specifying the corresponding covariant metric matrix.
- Use formulas shown thereafter that can only do analysis in the orthogonal coordinate system.

Python approach

Basic rules

In an orthogonal coordinate system,

- the metric tensor is a diagonal matrix;
- the basis vectors are mutually perpendicular, and the three covariant basis vectors are just parallel to their corresponding three contravariant basis vectors. For this reason, we often normalize basis vectors using Lamé coefficients, which ensures the normalized covariant vectors coincide with their corresponding contravariant basis vectors.

Vector notation

$$\vec{f} = F_i \hat{e}_i, \quad F_i = \hat{e}_i \cdot \vec{f} = f_i / h_i = h_i f^i, \quad (i = 1, 2, 3)
\overrightarrow{K} = K_{ij} \hat{e}_i \hat{e}_j, \quad K_{ij} = k_{ij} / (h_i h_j) = h_i h_j k^{ij}, \quad (i, j = 1, 2, 3)$$
(12)

Lamé coefficients

$$h_{1} = \sqrt{g_{11}} = \frac{1}{\sqrt{g^{11}}}, \quad h_{2} = \sqrt{g_{22}} = \frac{1}{\sqrt{g^{22}}}, \quad h_{3} = \sqrt{g_{33}} = \frac{1}{\sqrt{g^{33}}}$$

$$h_{i} = |\vec{e}_{i}| = \left[\left(\frac{\partial x}{\partial x^{i}} \right)^{2} + \left(\frac{\partial y}{\partial x^{i}} \right)^{2} + \left(\frac{\partial z}{\partial x^{i}} \right)^{2} \right]^{1/2}$$

$$= \left[\left(\frac{\partial x^{i}}{\partial x} \right)^{2} + \left(\frac{\partial x^{i}}{\partial y} \right)^{2} + \left(\frac{\partial x^{i}}{\partial z} \right)^{2} \right]^{-1/2}, \quad (i = 1, 2, 3)$$

$$\mathcal{J} = V = \sqrt{g} = h_{1}h_{2}h_{3}$$

$$\hat{e}_{i} = \frac{\vec{e}_{i}}{h_{i}} = h_{i}\vec{e}^{i}, \quad F_{i} = F^{i} = \frac{f_{i}}{h_{i}} = f^{i}h_{i}$$

$$(13)$$

Lamé coefficients [3] - Cont'd

Cylindrical coordinate				Spherical coordinate			
coordinate	r	θ	Z	coordinate	r	θ	φ
Lamé	1	r	1	Lamé	1	r	$r\sin\theta$
$\partial/\partial r$	0	1	0	$\partial/\partial r$	0	1	$\sin \theta$
$\partial/\partial\theta$	0	0	0	$\partial/\partial\theta$	0	0	$r\cos\theta$
$\partial/\partial z$	0	0	0	$\partial/\partial \varphi$	0	0	0
ê _i	êr	$\hat{e}_{ heta}$	ê _z	ê _i	ê _r	$\hat{m{e}}_{ heta}$	$\hat{\pmb{e}}_{m{arphi}}$
$\partial/\partial r$	0	0	0	$\partial/\partial r$	0	0	0
$\partial/\partial\theta$	$\hat{e}_{ heta}$	$-\hat{e}_r$	0	$\partial/\partial\theta$	$\hat{e}_{ heta}$	$-\hat{e}_r$	0
$\partial/\partial z$	0	0	0	$\partial/\partial \varphi$	$\sin heta \hat{m{e}}_{arphi}$	$\cos \theta \hat{e}_{\varphi}$	$-\sin\theta\hat{e}_r-\cos\theta\hat{e}_\theta$

Lengths

$$(ds)^{2} = (h_{1}dx^{1})^{2} + (h_{2}dx^{2})^{2} + (h_{3}dx^{3})^{2}$$

$$ds_{1} = h_{1}dx^{1}\hat{e}_{1}, \quad ds_{2} = h_{2}dx^{2}\hat{e}_{2}, \quad ds_{3} = h_{3}dx^{3}\hat{e}_{3}$$

$$da_{1} = h_{2}h_{3}dx^{2}dx^{3}\hat{e}_{1} \quad da_{2} = h_{1}h_{3}dx^{1}dx^{3}\hat{e}_{2} \quad da_{3} = h_{1}h_{2}dx^{1}dx^{2}\hat{e}_{3}$$

$$d\tau = Vdx^{1}dx^{2}dx^{3} = h_{1}h_{2}h_{3}dx^{1}dx^{2}dx^{3}$$

$$(14)$$

Differentiation of basis vectors

$$\nabla \cdot \hat{e}_{i} = \frac{1}{Vh_{i}} \frac{\partial V}{\partial x_{i}} - \frac{1}{h_{i}^{2}} \frac{\partial h_{i}}{\partial x_{i}} = \frac{1}{V} \frac{\partial}{\partial x_{i}} \left(\frac{V}{h_{i}}\right), \quad (i = 1, 2, 3)$$

$$\nabla \times \hat{e}_{i} = -h_{i} \nabla \left(\frac{1}{h_{i}}\right) \times \hat{e}_{i} = \frac{1}{h_{i}} \sum_{j=1}^{3} \left(\frac{1}{h_{j}} \frac{\partial h_{i}}{\partial x_{j}} \hat{e}_{j}\right) \times \hat{e}_{i}$$

$$(\hat{e}_{k} \cdot \nabla) \hat{e}_{i} = -\frac{1}{h_{k}} (\nabla h_{i}) \delta_{k}^{i} + \frac{1}{h_{i}h_{k}} \frac{\partial h_{k}}{\partial x_{i}} \hat{e}_{k}, \quad (i, k = 1, 2, 3)$$

$$\frac{\partial \hat{e}_{i}}{\partial x_{k}} = -(\nabla h_{i}) \delta_{k}^{i} + \frac{1}{h_{i}} \frac{\partial h_{k}}{\partial x_{i}} \hat{e}_{k} \quad (i, k = 1, 2, 3)$$

$$(15)$$

Differentiation of basis vectors-Cont'd

$$\begin{cases} (\hat{e}_{1} \cdot \nabla) \, \hat{e}_{1} = -\frac{1}{h_{1}} \nabla h_{1} + \frac{1}{h_{1}^{2}} \frac{\partial h_{1}}{\partial x_{1}} \hat{e}_{1} = -\frac{1}{h_{1}h_{2}} \frac{\partial h_{1}}{\partial x_{2}} \hat{e}_{2} - \frac{1}{h_{1}h_{3}} \frac{\partial h_{1}}{\partial x_{3}} \hat{e}_{3}, \\ (\hat{e}_{2} \cdot \nabla) \, \hat{e}_{2} = -\frac{1}{h_{2}} \nabla h_{2} + \frac{1}{h_{2}^{2}} \frac{\partial h_{2}}{\partial x_{2}} \hat{e}_{2} = -\frac{1}{h_{1}h_{2}} \frac{\partial h_{2}}{\partial x_{1}} \hat{e}_{1} - \frac{1}{h_{2}h_{3}} \frac{\partial h_{2}}{\partial x_{3}} \hat{e}_{3}, \\ (\hat{e}_{3} \cdot \nabla) \, \hat{e}_{3} = -\frac{1}{h_{3}} \nabla h_{3} + \frac{1}{h_{3}^{2}} \frac{\partial h_{3}}{\partial x_{3}} \hat{e}_{3} = -\frac{1}{h_{1}h_{3}} \frac{\partial h_{3}}{\partial x_{1}} \hat{e}_{1} - \frac{1}{h_{2}h_{3}} \frac{\partial h_{3}}{\partial x_{2}} \hat{e}_{2}. \end{cases}$$

$$(16)$$

$$\begin{cases}
\frac{\partial \hat{e}_{1}}{\partial x_{1}} = -\nabla h_{1} + \frac{1}{h_{1}} \frac{\partial h_{1}}{\partial x_{1}} \hat{e}_{1} = -\frac{1}{h_{2}} \frac{\partial h_{1}}{\partial x_{2}} \hat{e}_{2} - \frac{1}{h_{3}} \frac{\partial h_{1}}{\partial x_{3}} \hat{e}_{3} \\
\frac{\partial \hat{e}_{2}}{\partial x_{2}} = -\nabla h_{2} + \frac{1}{h_{2}} \frac{\partial h_{2}}{\partial x_{2}} \hat{e}_{2} = -\frac{1}{h_{1}} \frac{\partial h_{2}}{\partial x_{1}} \hat{e}_{1} - \frac{1}{h_{3}} \frac{\partial h_{2}}{\partial x_{3}} \hat{e}_{3} \\
\frac{\partial \hat{e}_{3}}{\partial x_{3}} = -\nabla h_{3} + \frac{1}{h_{3}} \frac{\partial h_{3}}{\partial x_{3}} \hat{e}_{3} = -\frac{1}{h_{1}} \frac{\partial h_{3}}{\partial x_{1}} \hat{e}_{1} - \frac{1}{h_{2}} \frac{\partial h_{3}}{\partial x_{2}} \hat{e}_{2}
\end{cases} (17)$$

Dot and cross product

$$\vec{a} \cdot \vec{b} = a^{i}b_{i} = \frac{A_{i}}{h_{i}}B_{i}h_{i} = A_{i}B_{i}$$

$$\vec{a} \cdot \vec{T} = A_{k}\hat{e}_{k} \cdot T_{ij}\hat{e}_{i}\hat{e}_{j} = A_{i}T_{ij}\hat{e}_{j}$$

$$\vec{T} \cdot \vec{a} = T_{ij}\hat{e}_{i}\hat{e}_{j} \cdot a_{k}\hat{e}_{k} = A_{j}T_{ij}\hat{e}_{i}$$

$$\vec{a} \times \vec{b} = A_{i}B_{i}\hat{e}_{i} \times \hat{e}_{i} = \epsilon_{ijk}A_{i}B_{i}\hat{e}_{k}$$

$$(18)$$

Gradient

$$\nabla \phi = \frac{\partial \phi}{\partial x^i} \vec{e}^i = \frac{1}{h_i} \frac{\partial \phi}{\partial x_i} \hat{e}_i \tag{19}$$

$$\hat{e}_i \cdot \nabla \phi = \frac{1}{h_i} \frac{\partial \phi}{\partial x_i} \tag{20}$$

$$\nabla \vec{u} = \hat{e}_{i}\hat{e}_{j}\frac{1}{h_{i}}\frac{\partial U_{j}}{\partial x^{i}} + \hat{e}_{i}\frac{\partial \hat{e}_{j}}{\partial x^{i}}\frac{U_{j}}{h_{i}} = \hat{e}_{i}\hat{e}_{j}\frac{1}{h_{i}}\frac{\partial U_{j}}{\partial x^{i}} + \hat{e}_{i}\frac{U_{j}}{h_{i}}\left(-(\nabla h_{j})\delta_{i}^{j} + \frac{1}{h_{j}}\frac{\partial h_{i}}{\partial x_{j}}\hat{e}_{i}\right)$$

$$= \hat{e}_{i}\hat{e}_{j}\frac{1}{h_{i}}\frac{\partial U_{j}}{\partial x^{i}} - \hat{e}_{i}\hat{e}_{k}\frac{U_{i}}{h_{i}}\frac{1}{h_{k}}\frac{\partial h_{i}}{\partial x_{k}} + \hat{e}_{i}\hat{e}_{i}\frac{U_{j}}{h_{i}}\frac{1}{h_{j}}\frac{\partial h_{i}}{\partial x_{j}}$$

$$(21)$$

Div

$$\nabla \cdot \vec{f} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} f^i \right) = \frac{1}{V} \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\frac{V F_i}{h_i} \right) \tag{22}$$

$$\nabla^2 \phi = \frac{1}{V} \frac{\partial}{\partial x_i} \left(\frac{V}{h_i^2} \frac{\partial \phi}{\partial x_i} \right) \tag{23}$$

$$\nabla \cdot \vec{\vec{T}} = \frac{1}{h_i} \frac{\partial T_{ik}}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{V} \frac{\partial (\frac{V}{h_i})}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{h_i} \frac{\partial \hat{e}_k}{\partial x_i}$$

$$= \frac{1}{h_i} \frac{\partial T_{ik}}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{V} \frac{\partial (\frac{V}{h_i})}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{h_i} \left[-(\nabla h_k) \delta_i^k + \frac{1}{h_k} \frac{\partial h_i}{\partial x_k} \hat{e}_i \right]$$

$$= \frac{1}{h_i} \frac{\partial T_{ik}}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{V} \frac{\partial (\frac{V}{h_i})}{\partial x_i} \hat{e}_k + \frac{T_{ik}}{h_i} \frac{1}{h_k} \frac{\partial h_i}{\partial x_k} \hat{e}_i - \frac{T_{ii}}{h_i} \frac{1}{h_i} \frac{\partial h_i}{\partial x_i} \hat{e}_j$$

$$(24)$$

Curl

$$\nabla \times \vec{f} = \frac{1}{\sqrt{g}} \frac{\partial f_i}{\partial x_j} \varepsilon_{kji} \vec{e}_k = \sum_{i,j,k=1}^{3} \frac{h_k}{V} \frac{\partial (h_i F_i)}{\partial x_j} \varepsilon_{kji} \hat{e}_k$$
 (25)

$$\nabla \times \vec{f} = \frac{1}{h_2 h_3} \left[\frac{\partial (h_3 F_3)}{\partial x_2} - \frac{\partial (h_2 F_2)}{\partial x_3} \right] \hat{e}_1 + \frac{1}{h_1 h_3} \left[\frac{\partial (h_1 F_1)}{\partial x_3} - \frac{\partial (h_3 F_3)}{\partial x_1} \right] \hat{e}_2 + \frac{1}{h_1 h_2} \left[\frac{\partial (h_2 F_2)}{\partial x_1} - \frac{\partial (h_1 F_1)}{\partial x_2} \right] \hat{e}_3$$
(26)

Laplacian

$$\nabla^{2}\phi = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^{j}} \left(g^{ij} \sqrt{g} \frac{\partial \phi}{\partial x^{i}} \right) = \frac{1}{V} \sum_{i=1}^{3} \frac{\partial}{\partial x_{i}} \left(\frac{V}{h_{i}^{2}} \frac{\partial \phi}{\partial x_{i}} \right)$$
(27)
$$\frac{1}{h_{i}h_{i}h_{i}} \left\{ \frac{\partial}{\partial x_{i}} \left(\frac{h_{2}h_{3}}{h_{3}} \frac{\partial \phi}{\partial x_{i}} \right) + \frac{\partial}{\partial x_{i}} \left(\frac{h_{1}h_{3}}{h_{3}} \frac{\partial \phi}{\partial x_{i}} \right) + \frac{\partial}{\partial x_{i}} \left(\frac{h_{1}h_{2}}{h_{3}} \frac{\partial \phi}{\partial x_{i}} \right) \right\}$$

$$\nabla^{2}\phi = \frac{1}{h_{1}h_{2}h_{3}} \left\{ \frac{\partial}{\partial x_{1}} \left(\frac{h_{2}h_{3}}{h_{1}} \frac{\partial \phi}{\partial x_{1}} \right) + \frac{\partial}{\partial x_{2}} \left(\frac{h_{1}h_{3}}{h_{2}} \frac{\partial \phi}{\partial x_{2}} \right) + \frac{\partial}{\partial x_{3}} \left(\frac{h_{1}h_{2}}{h_{3}} \frac{\partial \phi}{\partial x_{3}} \right) \right\}$$
(28)

The Python version OVA was implemented using the normalized vector notations shown before.

```
In [1]: import sys
          sys. path. append ("../")
          from OVA import *
          import sympy as sym
          sym, init printing()
In [2]: r = sym. Symbol('r', positive=True)
          t. z = sym. symbols('theta, z')
          cvlind = CoordinateSystem(r=r, t=t, p=z, coordinate='Cylindrical')
In [3]: # vector U
         Ur = sym. Function('U_r')(r, t, z); Ut = sym. Function('U_theta')(r, t, z); Uz = sym. Function('U_z')(r, t, z);
          U = [Ur. Ut. Uz]
          # scalar function phi
          phi = svm. Function('phi')(r, t, z)
          # 2-rank tensor T
          Trr = svm. Function('T (rr)')(r, t, z); Trt = sym. Function('T_(rt)')(r, t, z); Trz = sym. Function('T_(rz)')(r, t, z);
          Ttr = sym. Function('T_{tr}')(r, t, z): Ttt = sym. Function('T_{tr}')(r, t, z): Ttz = sym. Function('T_{tz}')(r, t, z):
          Tzr = sym. Function('T (zr)') (r, t, z); Tzt = sym. Function('T (zt)') (r, t, z); Tzz = sym. Function('T (zz)') (r, t, z);
          T = sym.Matrix([[Trr, Trt, Trz], [Ttr, Ttt, Ttz], [Tzr, Tzt, Tzz]])
          display(U)
          display(phi)
          display(T)
          [U_r(r, \theta, z), U_{\theta}(r, \theta, z), U_{\tau}(r, \theta, z)]
          \phi(r, \theta, z)
           T_{rr}(r, \theta, z) T_{rt}(r, \theta, z) T_{rz}(r, \theta, z)
            T_{tr}(r, \theta, z) = T_{tt}(r, \theta, z) = T_{tz}(r, \theta, z)
            T_{rr}(r, \theta, z) = T_{rt}(r, \theta, z) = T_{rr}(r, \theta, z)
```

Figure: Define coordinate system and variables

Parts of the benchmarks are shown here.

```
Grad of function \phi(r, \theta, z):
                                            \nabla \phi = \hat{e}_r \frac{\partial \phi}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial \phi}{\partial \theta} + \hat{e}_r \frac{\partial \phi}{\partial \theta}
In [4]: cylind.grad(phi)
 Out[4]: \left[\frac{\partial}{\partial r}\phi(r,\theta,z), \frac{\frac{\partial}{\partial \theta}\phi(r,\theta,z)}{r}, \frac{\partial}{\partial z}\phi(r,\theta,z)\right]
                                            Grad of vector \vec{u}:
                                                                                                                                                                                                   \nabla \vec{u} = \frac{\partial U_r}{\partial r} \hat{e}_r \hat{e}_r + \frac{\partial U_{\theta}}{\partial r} \hat{e}_r \hat{e}_{\theta} + \frac{\partial U_z}{\partial r} \hat{e}_r \hat{e}_z
                                                                                                                                                                                                                                                    +\left(\frac{1}{r}\frac{\partial U_r}{\partial \theta}-\frac{U_{\theta}}{r}\right)\hat{e}_{\theta}\hat{e}_r+\left(\frac{1}{r}\frac{\partial U_{\theta}}{\partial \theta}+\frac{U_r}{r}\right)\hat{e}_{\theta}\hat{e}_{\theta}+\frac{1}{r}\frac{\partial U_z}{\partial \theta}\hat{e}_{\theta}\hat{e}_z
                                                                                                                                                                                                                                                      +\frac{\partial U_r}{\partial z}\hat{e}_z\hat{e}_r + \frac{\partial U_\theta}{\partial z}\hat{e}_z\hat{e}_\theta + \frac{\partial U_z}{\partial z}\hat{e}_z\hat{e}_z
In [5]: cylind.grad(U)
Out[5]: \begin{bmatrix} \frac{\partial}{\partial r} U_{\Gamma}(r, \theta, z) & \frac{\partial}{\partial r} U_{\theta}(r, \theta, z) & \frac{\partial}{\partial r} U_{\theta}(r, \theta, z) \\ -U_{\theta}(r, \theta, z) + \frac{\partial}{\partial \theta} U_{\Gamma}(r, \theta, z) & \frac{\partial}{\partial \theta} U_{\theta}(r, \theta, z) & \frac{\partial}{\partial \theta} U_{\theta}(r, \theta, z) \\ -\frac{\partial}{\partial r} U_{\Gamma}(r, \theta, z) & \frac{\partial}{\partial r} U_{\theta}(r, \theta, z) & \frac{\partial}{\partial r} U_{\theta}(r, \theta, z) & \frac{\partial}{\partial r} U_{\Gamma}(r, \theta, z) \end{bmatrix}
```

Figure: Benchmark gradient operator

Vector \vec{u} dot the grad of \vec{u} :

$$\begin{split} \vec{u} \cdot \nabla \vec{u} &= \left[U_r \frac{\partial U_r}{\partial r} + U_\theta \left(\frac{1}{r} \frac{\partial U_r}{\partial \theta} - \frac{U_\theta}{r} \right) + U_z \frac{\partial U_z}{\partial z} \right] \hat{c}_r \\ &+ \left[U_r \frac{\partial U_\theta}{\partial r} + U_\theta \left(\frac{1}{r} \frac{\partial U_\theta}{\partial \theta} + \frac{U_r}{r} \right) + U_z \frac{\partial U_\theta}{\partial z} \right] \hat{c}_\theta \\ &+ \left[U_r \frac{\partial U_z}{\partial z} + U_\theta \frac{1}{r} \frac{\partial U_z}{\partial \theta} + U_z \frac{\partial U_z}{\partial z} \right] \hat{c}_z \end{split}$$

In [6]: cylind.dot(U, cylind.grad(U)) $\frac{\mathsf{Out} \{ \mathbf{6} \} :}{\mathsf{I}} \left[\frac{r \, \mathsf{U}_r \left(r, \theta, z \right) \frac{\partial}{\partial r} \, \mathsf{U}_r \left(r, \theta, z \right) + r \, \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_r \left(r, \theta, z \right) - \left(\mathsf{U}_\theta \left(r, \theta, z \right) - \frac{\partial}{\partial \theta} \, \mathsf{U}_r \left(r, \theta, z \right) \right) \, \mathsf{U}_\theta \left(r, \theta, z \right)}{\mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) + \mathsf{U}_z \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z \right) \frac{\partial}{\partial z} \, \mathsf{U}_\theta \left(r, \theta, z$ $\left. (r,\theta,z) + \frac{\mathrm{U}_{\theta}\left(r,\theta,z\right)\frac{\partial}{\partial\theta}\,\mathrm{U}_{\theta}\left(r,\theta,z\right)}{z},\;\mathrm{U}_{r}\left(r,\theta,z\right)\frac{\partial}{\partial r}\,\mathrm{U}_{z}\left(r,\theta,z\right) + \mathrm{U}_{z}\left(r,\theta,z\right)\frac{\partial}{\partial z}\,\mathrm{U}_{z}\left(r,\theta,z\right) + \frac{\mathrm{U}_{\theta}\left(r,\theta,z\right)\frac{\partial}{\partial\theta}\,\mathrm{U}_{z}\left(r,\theta,z\right)}{r}\right]$

Figure: Benchmark covariant derivative

Divergence of the tensor \overrightarrow{T}

$$\begin{split} \nabla \cdot \stackrel{\leftrightarrow}{T} &= \left[\frac{\partial}{r} \frac{\partial}{\partial r} (r T_{rr}) + \frac{1}{r} \frac{\partial T_{dr}}{\partial \theta} + \frac{\partial T_{zr}}{\partial z} - \frac{T_{d\theta}}{r} \right] \hat{\epsilon}_{r} \\ &+ \left[\frac{1}{r^{2}} \frac{\partial}{\partial r} (r^{2} T_{r\theta}) + \frac{1}{r} \frac{\partial T_{d\theta}}{\partial \theta} + \frac{\partial T_{z\theta}}{\partial z} - \frac{T_{r\theta} - T_{dr}}{r} \right] \hat{\epsilon}_{\theta} \\ &+ \left[\frac{1}{r} \frac{\partial}{\partial r} (r T_{zz}) + \frac{1}{r} \frac{\partial T_{d\theta}}{\partial z} + \frac{\partial T_{z\theta}}{\partial z} \right] \hat{\epsilon}_{z} \end{split}$$

In [8]: cylind.div(T) Out[8]: $\left[\frac{\partial}{\partial r} T_{rr}(r, \theta, z) + \frac{\partial}{\partial z} T_{rr}(r, \theta, z) + \frac{T_{rr}(r, \theta, z)}{r} - \frac{T_{tt}(r, \theta, z)}{r} + \frac{\frac{\partial}{\partial \theta} T_{rr}(r, \theta, z)}{r}, \frac{\partial}{\partial r} T_{rt}(r, \theta, z) + \frac{\partial}{\partial z} T_{rt}(r, \theta, z) + \frac{T_{rt}(r, \theta, z)}{r} + \frac{T_{tt}(r, \theta, z)$ $+\frac{\frac{\partial}{\partial \theta} T_{tt}(r, \theta, z)}{r}, \frac{\partial}{\partial r} T_{rz}(r, \theta, z) + \frac{\partial}{\partial z} T_{zz}(r, \theta, z) + \frac{T_{rz}(r, \theta, z)}{r} + \frac{\frac{\partial}{\partial \theta} T_{tz}(r, \theta, z)}{r}$

```
\vec{A} \times (\nabla \times \vec{B}) - \left[ \nabla \vec{B} \cdot \vec{A} - (\vec{A} \cdot \nabla) \vec{B} \right] = 0
```

```
In [7]: temp 1 = sym. Array(coord. cross(A, coord. curl(B)))
           temp_2 = sym. Array (coord. dot (coord. grad (B), A))
           temp_3 = sym. Array(coord. dot(A, coord. grad(B)))
           res = temp 1 - (temp 2 - temp 3)
           res.applyfunc(sym.simplify)
 Out[7]: [0 0 0]
           \nabla \cdot (\phi \vec{A}) - (\phi \nabla \cdot \vec{A} + \vec{A} \cdot \nabla \phi) = 0
In [8]: temp pA = [phi * k for k in A] # phi * |vec (A)
           sym. simplify(coord. div(temp pA) - (phi * coord. div(A) + coord. dot(A, coord. grad(phi))))
 Out[8]: 0
           \nabla \times (\phi \vec{A}) - (\phi \nabla \times \vec{A} + \nabla \phi \times \vec{A}) = 0
In [9]: temp pA = [phi * k for k in A]
           temp 1 = sym, Array(coord, curl(temp pA))
           temp 2 = svm. Arrav([phi * k for k in (coord. curl(A))])
           temp 3 = svm. Array(coord. cross(coord. grad(phi), A))
           svm.simplifv(temp 1 - (temp 2 + temp 3))
 Out[9]: [0 0 0]
```

Figure: Benchmark vector identities

Outline

Background Motivations Mathematics

Python approach introduction Mathematics Python version OVA

Mathematica approach introduction modify GVA package Mathematica version OVA

Summary

References

introduction

- Mathematica has (the most?) powerful symbolic calculation capability.
 - Mathematica is a functional programming language [7] in which there is no distinction between functions and data.
 - The rule-based programming makes the *Mathematica* highly suitable for the symbolic calculation.
 - Everything in *Mathematica* is an expression.
 - Every expressions can be decomposed into atoms (symbols, numbers, strings) and the rules attached to symbols (DownValues, UpValues, OwnValues, SubValues, NValues, FormatValues).
 - To define our own vector analysis package, we just attach new rules to symbols 'div', 'curl', ' ∇ ' and so on.

introduction

- First, we modified the GVA package of version 1.0 by Prof. Qin in 1997 to ensure its compatibility with *Mathematica* versions newer than 8.0, eliminating any associated warnings.
 - The Version 1.0 GVA and the popular current version of Mathematica (>8.0) have some non-essential conflicts, such as conflicts between GVA symbols and built-in symbols, which results in warnings when used.
 - The updates can be classified into two categories: 1. all functions in the package now have the Protected attribute and begin with lowercase letters to avoid conflicts with symbols in Symstem context. 2. Modifications in vectorNotation[] function are implemented to resolve issues with interpreting some of the notations such as ∇× and ∇·.
- Second, our *Mathematica* version OVA package is implemented based on the modified GVA package.

modify GVA package

```
Infalse SetDirectory[NotebookDirectory[1];
       Needs["Calculus`GeneralVectorAnalysis`", "GeneralVectorAnalysis.m"]
        Begin["Calculus`GeneralVectorAnalysis`"]
        Jacobian: Symbol Jacobian appears in multiple contexts (Calculus General/VectorAnalysis', System'); definitions in context Calculus General/VectorAnalysis' may shadow or be shadowed by other definitions.
        Grad: Symbol Grad appears in multiple contexts (Calculus' General/VectorAnalysis': System'): definitions in context Calculus' General/VectorAnalysis' may shadow or be shadowed by other definitions.
        Div: Symbol Div appears in multiple contexts (Calculus' General/VectorAnalysis', System'); definitions in context Calculus' General/VectorAnalysis' may shadow or be shadowed by other definitions.
        Curl: Symbol Curl appears in multiple contexts (Calculus General/VectorAnalysis'), System'); definitions in context Calculus General/VectorAnalysis' may shadow or be shadowed by other definitions.
        Laplacian: Symbol Laplacian appears in multiple contexts (Calculus'GeneralVectorAnalysis', System'); definitions in context Calculus'GeneralVectorAnalysis' may shadow or be shadowed by other definitions.
        UnitVector: Symbol UnitVector appears in multiple contexts {Calculus`GeneralVectorAnalysis`, System'}; definitions in context Calculus`GeneralVectorAnalysis' may shadow or be shadowed by other definitions.
        VectorQ: Symbol VectorQ appears in multiple contexts {Calculus GeneralVectorAnalysis', System'}; definitions in context Calculus GeneralVectorAnalysis' may shadow or be shadowed by other definitions.
        The Vector Calculus on General Coordinate is loaded in
       Use SetCoordinateSystem[ ] to set up a coordinate system
        The default CoordinateSystem is None
        Decrement: End is not a variable with a value, so its value cannot be changed.
        PreDecrement: End -- is not a variable with a value, so its value cannot be changed.
Out(=)= -- (End --)
Out[s]= Calculus GeneralVectorAnalysis
```

Figure: Warnings occur when importing the GVA version 1.0

■ Solution: all functions in the package now have the Protected attribute and begin with lowercase letters to avoid conflicts with symbols in Symstem' context.

modify GVA package

Figure: Errors occur when using some of the operator notations

■ Solution: modifications in Calculus'GeneralVectorAnalysis'vectorNotation[] function are implemented to resolve issues with interpreting some of the notations such as ∇× and ∇·.

Mathematica version OVA

- The *Mathematica* version OVA package is implemented based on the modified GVA package.
 - Vectors have 3 components with normalized basis vectors now (6 components before).
 - Every covariant and contravariant component is normalized using the Lamé coefficients.

$$\vec{f} = F_i \hat{e}_i, \quad F_i = \hat{e}_i \cdot \vec{f}$$

$$f_i = F_i h_i, \quad f^i = \frac{F_i}{h_i}$$
(29)

Mathematica version OVA: benchmark

```
In[1]:= SetDirectory[NotebookDirectory[11:
           Needs["OVA`", "OVA.m"]
           Begin["OVA"]
           The Vector Calculus on Orthogonal Coordinate is loaded in
          Use SetCoordinateSystem[] to set up a coordinate system
           The default CoordinateSystem is None
 Out[3]= OVA
  In[4]:= (*basic usage*)
  |n(S)| = \text{FullForm}/\Theta \{a \cdot (b+c), \forall \times (a+a \times (b \times c)), \forall \cdot (a+b \times d), (a \cdot \nabla), \nabla^2 f \nabla \cdot a, \hat{a}, |a|, \mathcal{T}[a] \}
 Out(S)= {dot(a, Plus(b, c)), curl(Plus(a, cross(a, cross(b, c)))), div(Plus(a, cross(b, d))),
            covariantDerivative[a, b], Times[div[a], laplacian[f]], unitVector[a], absoluteValue[a], jacobian[a]}
  in[6]:= declareVector[A, B0, B, C, D, F, G, H, J, ξ, Q]
           declareScalar[a, b, c, d, e, f, g, h]
           {A, B0, B, C, D, F, G, H, J, €, Q} are Vectors now.
           {a, b, c, d, e, f, g, h} are Scalars now.
  In[S] := \{A \times A, A \cdot (A \times C), \nabla \times (\nabla f), \nabla \cdot (\nabla \times A), \text{ vectorExpand}[A \times (B \times C)]\}
 Out[8]= {0, 0, 0, 0, -CA · B + BA · C}
  [n/9] = \text{vectorExpand} / (B \times C) + B \times (C \times A) + C \times (A \times B) \times (C \times D), \nabla \cdot (f(A \times B + \nabla \times C))
 Out[\Theta] = \{\emptyset, -DA \cdot (B \times C) + CA \cdot (B \times D), -fA \cdot (\nabla \times B) + fB \cdot (\nabla \times A) + (A \times B) \cdot (\nabla f) + (\nabla \times C) \cdot (\nabla f)\}
 In[10]:= (*an example from the ideal MHD*)
           Unprotect[div]; \nabla \cdot (B0) = 0; Protect[div]; O = \nabla \times (\varepsilon \times B0); J = \nabla \times O
Out[10]= -\nabla \times (\nabla \times (B\Theta \times \mathcal{E}))
Infilia vectorExpand[J]
Out[11]= \mathbf{B0} \times (\nabla (\nabla \cdot \mathcal{E})) + \nabla \times ((\mathbf{B0} \cdot \nabla) \mathcal{E}) - \nabla \times ((\mathcal{E} \cdot \nabla) \mathbf{B0}) - \nabla \times \mathbf{B0} \nabla \cdot \mathcal{E}
```

Figure: The coordinate-independent vector analysis provided by OVA here is equivalent to GVA

Mathematica version OVA: benchmark

```
In[23]:= \nabla^2 phi[r, \theta, z] // Assuming[r > \theta, FullSimplify[#] // Expand] &
Out[23] = phi^{(\theta,\theta,2)} [r,\theta,z] + \frac{phi^{(\theta,2,\theta)} [r,\theta,z]}{2} + \frac{phi^{(1,\theta,\theta)} [r,\theta,z]}{2} + phi^{(2,\theta,\theta)} [r,\theta,z]
    In[24]:= An = defineVector[Ar[r, 0, z], At[r, 0, z], Az[r, 0, z]]
Out[24]= vector[\{Ar[r, \theta, z], At[r, \theta, z], Az[r, \theta, z]\}]
      In[25]:= (A<sub>0</sub> · ∇) A<sub>0</sub> // Assuming[r > 0, FullSimplify[#] // Expand] &
\text{Out} [2S] = \text{Vector} \Big[ \Big\{ \frac{-\text{At}[\textbf{r}, \theta, \textbf{z}]^2 + \text{rAz}[\textbf{r}, \theta, \textbf{z}] \; \text{Ar}^{(\theta, \theta, \textbf{1})} \left[\textbf{r}, \theta, \textbf{z}\right] + \text{At}[\textbf{r}, \theta, \textbf{z}] \; \text{Ar}^{(\theta, \textbf{1}, \theta)} \left[\textbf{r}, \theta, \textbf{z}\right] + \text{rAr}[\textbf{r}, \theta, \textbf{z}] \; \text{Ar}^{(\textbf{1}, \theta, \theta)} \left[\textbf{r}, \theta, \textbf{z}\right] + \text{rAr}[\textbf{r}, \theta, \textbf{z}] \; \text{Ar}^{(\textbf{1}, \theta, \theta)} \left[\textbf{r}, \theta, \textbf{z}\right] + \text{rAr}[\textbf{r}, \theta, \textbf{z}] +
                                                \text{Az}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right]\,\text{At}^{\left(\theta,\theta,1\right)}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right] + \frac{\text{At}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right]\,\left(\text{Ar}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right]+\text{At}^{\left(\theta,1,\theta\right)}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right]\right)}{2} + \text{Ar}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right]\,\text{At}^{\left(1,\theta,\theta\right)}\left[\textbf{r},\,\boldsymbol{\theta},\,\textbf{z}\right], 
                                               \text{Az[r, $\theta$, $z$] Az$}^{(\theta,\theta,1)}\left[r, \; \theta, \; z\right] + \frac{\text{At[r, $\theta$, $z$] Az$}^{(\theta,1,\theta)}\left[r, \; \theta, \; z\right]}{r} + \text{Ar[r, $\theta$, $z$] Az$}^{(1,\theta,\theta)}\left[r, \; \theta, \; z\right]\Big\}\Big]
    In[26]:= \nabla \cdot A_0 // Assuming[r > 0, FullSimplify[#] // Expand] &
Out[26] = \frac{Ar[r, \theta, z]}{r} + Az^{(\theta,\theta,1)}[r, \theta, z] + \frac{At^{(\theta,1,\theta)}[r, \theta, z]}{r} + Ar^{(1,\theta,\theta)}[r, \theta, z]
    ln[27] = \nabla \times A_0 // Assuming[r > 0, FullSimplify[#] // Expand] &
 \text{Out}(27) = \text{vector} \left[ \left\{ -\text{At}^{(\theta,\theta,1)} \left[ r, \theta, z \right] + \frac{\text{Az}^{(\theta,1,\theta)} \left[ r, \theta, z \right]}{2}, \text{Ar}^{(\theta,\theta,1)} \left[ r, \theta, z \right] - \text{Az}^{(1,\theta,\theta)} \left[ r, \theta, z \right], \frac{\text{At} \left[ r, \theta, z \right] - \text{Ar}^{(\theta,1,\theta)} \left[ r, \theta, z \right]}{2} + \text{At}^{(1,\theta,\theta)} \left[ r, \theta, z \right] \right\} \right] 
    In[28] - VAo // Assuming[r > 0. FullSimplify[#] // Expand] &
\text{Out}[28] = \left\{ \left\{ \text{Ar}^{(1,\theta,\theta)}\left[\text{r,}\ \theta,\ \text{z}\right],\, \text{At}^{(1,\theta,\theta)}\left[\text{r,}\ \theta,\ \text{z}\right],\, \text{Az}^{(1,\theta,\theta)}\left[\text{r,}\ \theta,\ \text{z}\right] \right\}, \right.
                                         \left\{-\frac{At[r,\theta,z]}{r}+\frac{Ar^{(\theta,1,\theta)}[r,\theta,z]}{r},\frac{Ar[r,\theta,z]}{r}+\frac{At^{(\theta,1,\theta)}[r,\theta,z]}{r},\frac{Az^{(\theta,1,\theta)}[r,\theta,z]}{r},\frac{Az^{(\theta,1,\theta)}[r,\theta,z]}{r}\right\},\\ \left\{Ar^{(\theta,\theta,1)}[r,\theta,z],At^{(\theta,\theta,1)}[r,\theta,z],Az^{(\theta,\theta,1)}[r,\theta,z]\right\}
    In[29]:= V • V × Ao
Out[29]= 0
```

Figure: Some of the vector analysis operations in the cylindrical coordinate system have been benchmarked

Outline

Background

Motivations

Mathematics

Python approach

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Mathematics
Python version OVA

Mathematica approach

introduction modify GVA package *Mathematica* version OVA

Summary

References

Summary

- The OVA (Orthogonal curvilinear coordinate Vector Analysis) package has been implemented in both Python and Mathematica versions.
 - The Python version OVA is implemented using the vector analysis formulas assuming the basis normalized by the Lamé coefficients (thus can only be used in orthogonal coordinates).
 - The GVA package, originally developed by Prof. Qin in 1997, has been modified to ensure compatibility with newer versions of Mathematica, beyond version 8.0.
 - The Mathematica version of the OVA package is built upon the modified GVA package, which includes updated vector definitions and the normalization of each component using Lamé coefficients.
- The formulas used by OVA are presented, which can serve as a helpful cheatsheet. Additionally, formulas specific to cylindrical coordinates are listed in the 'Backup' section, which may be useful for those interested in linear devices.

References I

- [1] Hong Qin, WM Tang, and G Rewoldt. "Symbolic vector analysis in plasma physics". In: *Computer physics communications* 116.1 (1999), pp. 107–120.
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https://github.com/ymma98/0VA.git

All the codes are avaliable on Github. Welcome issues and pull requests!

Thank You for Your Attention!

- The application of vector analysis in cylindrical coordinates is particularly useful for FRC research (which is important for me).
- I list the formulas in the cylindrical coordinate system (r, θ, z) separately here for easy use.

$$h_1 = 1$$
 $h_2 = r$ $h_3 = 1$ (30)

$$\mathcal{J} = V = \sqrt{g} = h_1 h_2 h_3 = r \tag{31}$$

$$\vec{a} \cdot \vec{b} = a^{i}b_{i} = \frac{A_{i}}{h_{i}}B_{i}h_{i} = A_{i}B_{i}$$

$$\vec{a} \cdot \vec{T} = A_{k}\hat{e}_{k} \cdot T_{ij}\hat{e}_{i}\hat{e}_{j} = A_{i}T_{ij}\hat{e}_{j}$$

$$\vec{T} \cdot \vec{a} = T_{ij}\hat{e}_{i}\hat{e}_{j} \cdot a_{k}\hat{e}_{k} = A_{j}T_{ij}\hat{e}_{i}$$

$$\vec{a} \times \vec{b} = A_{i}B_{j}\hat{e}_{i} \times \hat{e}_{j} = \epsilon_{ijk}A_{i}B_{j}\hat{e}_{k}$$

$$(32)$$

$$\vec{a} \times \vec{b} = \hat{e}_r (A_\theta B_z - A_z B_\theta) + \hat{e}_\theta (A_z B_r - A_r B_z) + \hat{e}_z (A_r B_\theta - A_\theta B_r) \quad (33)$$

$$\vec{a} \cdot \vec{b} = a^{i}b_{i} = \frac{A_{i}}{h_{i}}B_{i}h_{i} = A_{i}B_{i}$$

$$\vec{a} \cdot \vec{T} = A_{k}\hat{e}_{k} \cdot T_{ij}\hat{e}_{i}\hat{e}_{j} = A_{i}T_{ij}\hat{e}_{j}$$

$$\vec{T} \cdot \vec{a} = T_{ij}\hat{e}_{i}\hat{e}_{j} \cdot a_{k}\hat{e}_{k} = A_{j}T_{ij}\hat{e}_{i}$$

$$\vec{a} \times \vec{b} = A_{i}B_{j}\hat{e}_{i} \times \hat{e}_{j} = \epsilon_{ijk}A_{i}B_{j}\hat{e}_{k}$$

$$(34)$$

$$\vec{a} \times \vec{b} = \hat{e}_r (A_\theta B_z - A_z B_\theta) + \hat{e}_\theta (A_z B_r - A_r B_z) + \hat{e}_z (A_r B_\theta - A_\theta B_r)$$
 (35)

$$\nabla \cdot \hat{e}_r = \frac{1}{r}$$

$$\nabla \cdot \hat{e}_\theta = 0$$

$$\nabla \cdot \hat{e}_z = 0$$

$$\nabla \times \hat{e}_r = 0$$
(36)

$$\nabla \times \hat{\mathbf{e}}_{\theta} = \frac{1}{r} \tag{37}$$

$$\nabla \times \hat{\mathbf{e}}_{\mathbf{z}} = 0$$

$$\begin{cases} (\hat{e}_r \cdot \nabla) \, \hat{e}_r = 0 \\ (\hat{e}_\theta \cdot \nabla) \, \hat{e}_\theta = -\frac{1}{r} \hat{e}_r \\ (\hat{e}_z \cdot \nabla) \, \hat{e}_z = 0 \end{cases}$$
(38)

$$\begin{cases}
\frac{\partial \hat{\mathbf{e}}_r}{\partial f} = 0 \\
\frac{\partial \hat{\mathbf{e}}_{\theta}}{\partial \theta} = -\hat{\mathbf{e}}_r \\
\frac{\partial \hat{\mathbf{e}}_z}{\partial r} = 0
\end{cases}$$
(39)

$$\nabla = \vec{e}^i \frac{\partial}{\partial x^i} = \hat{e}_i \frac{1}{h_i} \frac{\partial}{\partial x^i} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_z \frac{\partial}{\partial z}$$

$$\nabla^2 = \Delta = \frac{1}{V} \sum_{i=1}^3 \frac{\partial}{\partial x_i} \left(\frac{V}{h_i^2} \frac{\partial}{\partial x_i} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}$$

$$\vec{u} \cdot \nabla = U_i \hat{e}_i \cdot \hat{e}_j \frac{1}{h_j} \frac{\partial}{\partial x^j} = U_i \frac{1}{h_i} \frac{\partial}{\partial x^i} = U_r \frac{\partial}{\partial r} + \frac{U_\theta}{r} \frac{\partial}{\partial \theta} + U_z \frac{\partial}{\partial z}$$
(40)

$$\nabla \phi = \hat{\mathbf{e}}_r \frac{\partial \phi}{\partial r} + \hat{\mathbf{e}}_\theta \frac{1}{r} \frac{\partial \phi}{\partial \theta} + \hat{\mathbf{e}}_z \frac{\partial \phi}{\partial z}$$

$$\nabla \cdot \vec{U} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} U^i \right) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \left(\sqrt{g} \frac{U^i}{h_i} \right) = \frac{1}{r} \frac{\partial}{\partial r} (r U_r) + \frac{1}{r} \frac{\partial U_{\theta}}{\partial \theta} + \frac{\partial U_z}{\partial z}$$

$$\nabla \times \vec{u} = \frac{1}{h_i} \sum_{j=1}^{3} \left(\frac{1}{h_j} \frac{\partial h_i}{\partial x_j} \hat{e}_j \right) \times \hat{e}_i$$

$$= \left(\frac{1}{r} \frac{\partial U_z}{\partial \theta} - \frac{\partial U_{\theta}}{\partial z} \right) \hat{e}_r + \left(\frac{\partial U_r}{\partial z} - \frac{\partial U_z}{\partial r} \right) \hat{e}_{\theta} + \left[\frac{1}{r} \frac{\partial}{\partial r} (rU_{\theta}) - \frac{1}{r} \frac{\partial U_r}{\partial \theta} \right] \hat{e}_z$$
(41)

$$\nabla \vec{u} = \hat{e}_{i} \hat{e}_{j} \frac{1}{h_{i}} \frac{\partial U_{j}}{\partial x^{i}} + \hat{e}_{i} \frac{\partial \hat{e}_{j}}{\partial x^{i}} \frac{U_{j}}{h_{i}} = \frac{\partial U_{r}}{\partial r} \hat{e}_{r} \hat{e}_{r} + \frac{\partial U_{\theta}}{\partial r} \hat{e}_{r} \hat{e}_{\theta} + \frac{\partial U_{z}}{\partial r} \hat{e}_{r} \hat{e}_{z}$$

$$+ \left(\frac{1}{r} \frac{\partial U_{r}}{\partial \theta} - \frac{U_{\theta}}{r} \right) \hat{e}_{\theta} \hat{e}_{r} + \left(\frac{1}{r} \frac{\partial U_{\theta}}{\partial \theta} + \frac{U_{r}}{r} \right) \hat{e}_{\theta} \hat{e}_{\theta} + \frac{1}{r} \frac{\partial U_{z}}{\partial \theta} \hat{e}_{\theta} \hat{e}_{z}$$

$$+ \frac{\partial U_{r}}{\partial z} \hat{e}_{z} \hat{e}_{r} + \frac{\partial U_{\theta}}{\partial z} \hat{e}_{z} \hat{e}_{\theta} + \frac{\partial U_{z}}{\partial z} \hat{e}_{z} \hat{e}_{z}$$

$$\vec{u} \cdot \nabla \vec{u} = \left[U_{r} \frac{\partial U_{r}}{\partial r} + U_{\theta} \left(\frac{1}{r} \frac{\partial U_{r}}{\partial \theta} - \frac{U_{\theta}}{r} \right) + U_{z} \frac{\partial U_{r}}{\partial z} \right] \hat{e}_{r}$$

$$+ \left[U_{r} \frac{\partial U_{\theta}}{\partial r} + U_{\theta} \left(\frac{1}{r} \frac{\partial U_{\theta}}{\partial \theta} + \frac{U_{r}}{r} \right) + U_{z} \frac{\partial U_{\theta}}{\partial z} \right] \hat{e}_{\theta}$$

$$+ \left[U_{r} \frac{\partial U_{z}}{\partial r} + U_{\theta} \frac{1}{r} \frac{\partial U_{z}}{\partial \theta} + U_{z} \frac{\partial U_{z}}{\partial z} \right] \hat{e}_{z}$$

$$\nabla \cdot \vec{T} = \left[\frac{1}{r} \frac{\partial}{\partial r} (r T_{rr}) + \frac{1}{r} \frac{\partial T_{\theta r}}{\partial \theta} + \frac{\partial T_{zr}}{\partial z} - \frac{T_{\theta \theta}}{r} \right] \hat{e}_{r}$$

$$+ \left[\frac{1}{r^{2}} \frac{\partial}{\partial r} (r^{2} T_{r\theta}) + \frac{1}{r} \frac{\partial T_{\theta \theta}}{\partial \theta} + \frac{\partial T_{zz}}{\partial z} - \frac{T_{r\theta} - T_{\theta r}}{r} \right] \hat{e}_{\theta}$$

$$+ \left[\frac{1}{r} \frac{\partial}{\partial r} (r T_{rz}) + \frac{1}{r} \frac{\partial T_{\theta z}}{\partial \theta} + \frac{\partial T_{zz}}{\partial z} \right] \hat{e}_{z}$$