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PARTIAL DIFFERENTIAL EQUATIONS IN THE PHYSICAL DOMAIN

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ABSTRACT

Partial differential equations in the physical domain Xn can be solved on a structured numerical grid obtained by mapping a reference grid in the logical region Ξn into Xn with a coordinate transformation

$$x(\xi) : \Xi n \rightarrow Xn.$$

The structured grid concept also gives an alternative way to obtain a numerical solution to a partial differential equation, by solving the transformed equation with respect to the new independent variables ξi on the reference grid in the logical domain Ξn.

Some notions and relations concerning the coordinate transformations yielding structured grids are discussed in this chapter. These notions and relations are used to represent some conservation-law equations in the new logical coordinates in a convenient form. This article highlights the numerical solution of partial differential equations.

KEYWORDS:

Partial Differential Equation , Numerical, Equation

INTRODUCTION

The numerical solution of equations requires the application of moving grids and the corresponding coordinate transformations, which are dependent on time. Commonly, such coordinate transformations are determined in the form of a vector-valued time-dependent function

$$x(t,\xi) : \Xi^n \to X_t^n, \quad \xi \in \Xi^n,\ t \in [0,1],$$

where the variable t represents the time and Xn t is an n-dimensional domain whose boundary points change smoothly with respect to t.

It is assumed that x(t, ξ) is sufficiently smooth with respect to ξi and t and, in addition, that it is invertible for all t ∈ [0, 1]. Therefore there is also the time-dependent inverse transformation

$$\xi(t, x) : X_t^n \to \Xi^n$$

for every t ∈ [0, 1].

The introduction of these time-dependent coordinate transformations enables one to compute an unsteady solution on a fixed uniform grid in Ξn by the numerical solution of the transformed equations.

Many physical problems are modeled in the form of non-stationary conservation-law equations which include the time derivative. The formulas can be used directly, by transforming the equations at every value of time t.

However, such utilization of the formulas does not influence the temporal derivative, which is transformed simply to the form

$$\frac{\partial}{\partial t} + \frac{\partial \xi^i}{\partial t} \frac{\partial}{\partial \xi^i}, \quad i = 1, \ldots, n,$$

so that does not maintain the property of divergency and its coefficients are not derived from the elements of the metric tensor.

The first derivative xτ , x = (x1, x2,...,xn), of the transformation x(ξ,τ) has a clear physical interpretation as the velocity vector of grid point movement.

Let the vector xτ , in analogy with the flow velocity vector u, be designated by w = (w1,...,wn), i.e. wi = xi τ . The ith component wi of the vector wi in the tangential bases xξi , i = 1, . . . , n, is expressed

$$\overline{w}^i = w^j \frac{\partial \xi^i}{\partial x^j} = \frac{\partial x^j}{\partial \tau} \frac{\partial \xi^i}{\partial x^j}, \quad i, j = 1, \ldots, n.$$

Therefore

$$\boldsymbol{w} = \overline{w}^i \boldsymbol{x}_{\xi^i}, \quad i = 1, \ldots, n,$$

i.e.

$$w^i = \frac{\partial x^i}{\partial \tau} = \overline{w}^j \frac{\partial x^i}{\partial \xi^j}, \quad i, j = 1, \ldots, n.$$

Differentiation with respect to ξ^0 of the composition of $\boldsymbol{x}_0(\boldsymbol{\xi}_0)$ a
yields

$$\frac{\partial \xi^i}{\partial x^0} \frac{\partial x^0}{\partial \xi^0} + \frac{\partial \xi^i}{\partial x^j} \frac{\partial x^j}{\partial \xi^0} = 0, \quad i, j = 1, \ldots, n.$$

Therefore we obtain the result

$$\frac{\partial \xi^i}{\partial t} = -\frac{\partial x^j}{\partial \tau} \frac{\partial \xi^i}{\partial x^j} = -\overline{w}^i, \quad i, j = 1, \ldots, n.$$

It is apparent that the Jacobians of the coordinate transformations x(τ, ξ) and x0(ξ0) coincide, i.e.

$$\det\left(\frac{\partial x^i}{\partial \xi^j}\right) = \det\left(\frac{\partial x^k}{\partial \xi^l}\right) = J, \quad i,j = 0,1,\ldots,n, \; k,l = 1,\ldots,n.$$

$$\boldsymbol{x}_0(\boldsymbol{\xi}_0) : \Xi^{n+1} \to X^{n+1}$$

is expressed by the relation

$$\frac{1}{J}\frac{\partial}{\partial \xi^i}J = \frac{\partial^2 x^k}{\partial \xi^i \partial \xi^m}\frac{\partial \xi^m}{\partial x^k}, \quad i,k,m = 0,1,\ldots,n,$$

$$\frac{1}{J}\frac{\partial}{\partial \tau}J = \frac{\partial}{\partial \xi^m}\left(\frac{\partial x^k}{\partial \tau}\right)\frac{\partial \xi^m}{\partial x^k} = \mathrm{div}_x \frac{\partial \boldsymbol{x}}{\partial \tau}, \quad k,m = 0,1,\ldots,n,$$

and, taking into account (2.84),

$$\begin{aligned}\frac{1}{J}\frac{\partial}{\partial \tau}J &= \frac{\partial}{\partial \xi^m}\left(\overline{w}^j\frac{\partial x^k}{\partial \xi^j}\right)\frac{\partial \xi^m}{\partial x^k}\\ &= \frac{\partial \overline{w}^m}{\partial \xi^m} + \overline{w}^i\frac{\partial^2 x^k}{\partial \xi^j \partial \xi^m}\frac{\partial \xi^m}{\partial x^k}, \quad j,k,m = 1,\ldots,n.\end{aligned}$$

$$\frac{\partial}{\partial \xi^j}\left(J\frac{\partial \xi^j}{\partial x^i}\right) = 0, \quad i,j = 0,1,\ldots,n.$$

Therefore for $i = 0$ we obtain

$$\frac{\partial}{\partial \tau}(J) + \frac{\partial}{\partial \xi^j}\left(J\frac{\partial \xi^j}{\partial t}\right) = 0, \quad j = 1,\ldots,n,$$

and, taking into account (2.85),

$$\frac{\partial}{\partial \tau}J - \frac{\partial}{\partial \xi^j}(J\overline{w}^j) = 0, \quad j = 1,\ldots,n,$$

One of the most popular systems of coordinates in fluid dynamics is the Lagrangian system.

A coordinate ξi is Lagrangian if the both the ith component of the flow velocity vector u and the grid velocity w in the tangent basis $x\xi j$, j = 1,...,m, coincide,

i.e. ui − wi = 0.

RESEARCH STUDY

Conservation-law equations in curvilinear coordinates are typically deduced from the equations in Cartesian coordinates through the classical formulas of tensor calculus, by procedures which include the substitution of tensor derivatives for ordinary derivatives. The formulation and evaluation of the tensor derivatives is rather difficult, and they retain some elements of mystery.

However, these derivatives are based on specific transformations of tensors, modeling in the equations some dependent variables, e.g. the components of a fluid velocity vector, which after the transformation have a clear interpretation in terms of the contra-variant components of the vector. With this concept, the conservation-law equations are readily written out in this chapter without application of the tensor derivatives, but utilizing instend only some specific transformations of the dependent variables, ordinary derivatives, and one basic identity of coordinate transformations derived from the formula for differentiation of the Jacobian.

For generality, the transformations of the coordinates are mainly considered for arbitrary n-dimensional domains, though in practical applications the dimension n equals 1, 2, 3, or 4 for time-dependent transformations of three dimensional domains.

We also apply chiefly a standard vector notation for the coordinates, as variables with indices. Sometimes, however, particularly in figures, the ordinary designation for three-dimensional coordinates, namely x, y, z for the physical coordinates and ξ,η,ζ for the logical ones, is used to simplify the presentation.

Let x(ξ) : Ξn → Xn, ξ = (ξ1,...,ξn), x = (x1,...,xn), be a smooth invertible coordinate transformation of the physical region Xn ⊂ Rn from the parametric domain Ξn ⊂ Rn. If Ξn is a standard logical domain, then, in accordance with Chap. 1, this coordinate transformation can be used to generate a structured grid in Xn.

Here and later Rn presents the Euclidean space with the Cartesian basis e1,..., en, which represents an orthogonal system of vectors, i.e.

$$\boldsymbol{e}_i \cdot \boldsymbol{e}_j = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

Thus we have

$$\boldsymbol{x} = x^1 \boldsymbol{e}_1 + \cdots + x^n \boldsymbol{e}_n,$$
$$\boldsymbol{\xi} = \xi^1 \boldsymbol{e}_1 + \cdots + \xi^n \boldsymbol{e}_n.$$

The values xi , i = 1, . . . , n, are called the Cartesian coordinates of the vector x. The coordinate transformation x(ξ) defines, in the domain Xn, new coordinates ξ1,...,ξn, which are called the curvilinear coordinates.

This transformation can be considered analogously as a mapping introducing a curvilinear coordinate system x1,...,xn in the domain Ξn ⊂ Rn.

$$\frac{\partial \xi^i}{\partial x^j} = (-1)^{i+j} \frac{\partial x^{3-j}}{\partial \xi^{3-i}} \Big/ J,$$
$$\frac{\partial x^i}{\partial \xi^j} = (-1)^{i+j} J \frac{\partial \xi^{3-j}}{\partial x^{3-i}}, \quad i, j = 1, 2.$$

Similar relations between the elements of the corresponding three-dimens matrices have the form

$$\frac{\partial \xi^i}{\partial x^j} = \frac{1}{J}\left(\frac{\partial x^{j+1}}{\partial \xi^{i+1}}\frac{\partial x^{j+2}}{\partial \xi^{i+2}} - \frac{\partial x^{j+1}}{\partial \xi^{i+2}}\frac{\partial x^{j+2}}{\partial \xi^{i+1}}\right),$$
$$\frac{\partial x^i}{\partial \xi^j} = J\left(\frac{\partial \xi^{j+1}}{\partial x^{i+1}}\frac{\partial \xi^{j+2}}{\partial x^{i+2}} - \frac{\partial \xi^{j+1}}{\partial x^{i+2}}\frac{\partial \xi^{j+2}}{\partial x^{i+1}}\right), \quad i, j = 1, 2, 3,$$

Thus the cells in the domain Xn whose edges are formed by the vectors $hx_{\xi i}$, $i = 1, \ldots, n$, are approximately the same as those obtained by mapping the uniform coordinate cells in the computational domain Ξn with the transformation $x(\xi)$.

Consequently, the uniformly contracted parallelepiped spanned by the tangential vectors $x_{\xi i}$, $i = 1, \ldots, n$, represents to a high order of accuracy with respect to h the cell of the coordinate grid at the corresponding point in Xn.

In particular, for the length li of the ith grid edge

we have

$$li = h|x\xi i| + O(h2).$$

The volume Vh (area in two dimensions) of the cell is expressed as follows:

$$Vh = hnV + O(hn+1),$$

where V is the volume of the n-dimensional parallelepiped determined by the tangential vectors $x_{\xi i}$, $i = 1, \ldots, n$.

The tangential vectors $x_{\xi i}$, $i = 1, \ldots, n$, are called the base covariant vectors since they comprise a vector basis.

The sequence $x_{\xi 1}$,..., $x_{\xi n}$ of the tangential vectors has a right-handed orientation if the Jacobian of the transformation $x(\xi)$ is positive.

Otherwise, the base vectors $x_{\xi i}$ have a left-handed orientation. The operation of the dot product on these vectors produces elements of the covariant metric tensor.

These elements generate the coefficients that appear in the transformed governing equations that model the conservation-law equations of mechanics. Besides this, the metric elements play a primary role in studying and formulating various geometric characteristics of the grid cells.

The elements of the covariant and contravariant metric tensors are defined by the dot products of the base tangential and normal vectors, respectively. These elements are suitable for describing the internal features of the cells such as the lengths of the edges, the areas of the faces, their volumes, and the angles between the edges and the faces.

However, as they are derived from the first derivatives of the coordinate transformation $x(\xi)$, the direct use of the metric elements is not sufficient for the description of the dynamic features of the grid (e.g. curvature), which reflect changes between adjacent cells. This is because the formulation of these grid features relies not only on the first derivatives but also on the second derivatives of $x(\xi)$. Therefore there is a need to study relations connected with the second derivatives of the coordinate parametrizations.

This presents some notations and formulas which are concerned with the second derivatives of the components of the coordinate transformations. These notations and relations will be used to describe the curvature and eccentricity of the coordinate lines and to formulate some equations of mechanics in new independent variables.

SIGNIFICANCE OF THE STUDY

The edge of a grid cell in the ξi direction can be represented with high accuracy by the base vector $x\xi i$ contracted by the factor h, which represents the step size of a uniform grid in Ξn. Therefore the local change of the edge in the ξj direction is characterized by the derivative of $x\xi i$ with respect to ξj , i.e. by $x\xi i\xi j$.

Since the second derivatives may be used to formulate quantitative measures of the grid, we describe these vectors $x\xi i\xi j$ through the base tangential and normal vectors using certain three-index quantities known as Christoffel symbols.

The Christoffel symbols are commonly used in formulating measures of the mutual interaction of the cells and in formulas for differential equations.

Let us denote by Γk ij the kth contravariant component of the vector xξiξj in the base tangential vectors xξk , k = 1, . . . , n. The superscript k in this designation relates to the base vector xξk and the subscript ij corresponds to the mixed derivative with respect to ξi and ξj .

Thus

$$\boldsymbol{x}_{\xi^i \xi^j} = \Gamma^k_{ij} \boldsymbol{x}_{\xi^k}, \quad i, j, k = 1, \dots, n,$$

and consequently

$$\frac{\partial^2 x^p}{\partial \xi^j \partial \xi^k} = \Gamma^m_{kj} \frac{\partial x^p}{\partial \xi^m}, \quad j, k, m, p = 1, \dots, n.$$

The examples of gas-dynamics equations described above, which include the terms wi , allow one to obtain the equations in Lagrange coordinates by substituting ui for wi in the written-out equations in accordance with the relation.

In such a manner, we obtain the equation of mass conservation, for example, in the Lagrangian coordinates ξ1,...,ξn as

$$\frac{\partial J\rho}{\partial \tau} = JF$$

$$\frac{\partial}{\partial \tau}(J\rho\phi) + \frac{\partial}{\partial \xi^j}\left(Jg^{kj}\epsilon\frac{\partial \phi}{\partial \xi^k}\right) = JS, \quad j, k = 1, \dots, n,$$

and

$$\frac{\partial}{\partial \tau}\left[J\rho\left(e + \frac{1}{2}g_{mk}\overline{u}^m\overline{u}^k\right)\right] + \frac{\partial}{\partial \xi^j}(J\overline{pu}^j) = J\rho g_{mk}\overline{f}^m\overline{u}^k, \quad j, m, k = 1, 2, 3,$$

Many of the basic formulations of vector calculus and tensor analysis may be found in the books by Kochin (1951), Sokolnikoff (1964) and Gurtin (1981). The formulation of general metric and tensor concepts specifically aimed at grid generation was originally performed by Eiseman (1980) and Warsi (1981). Very important applications of the most general tensor relations to the formulation of unsteady equations in curvilinear coordinates in a strong conservative form were presented by Vinokur (1974).

$$\begin{aligned}
\overline{A}^{ij} &= A^{km}\frac{\partial \xi^i}{\partial x^k}\frac{\partial \xi^j}{\partial x^m}, && i,j,m,n=1,\dots,n,\\
\Gamma^i_{kj} &= \frac{\partial^2 x^l}{\partial \xi^k \partial \xi^j}\frac{\partial \xi^i}{\partial x^l}, && i,j,k,l=1,\dots,n,\\
\overline{F}^i &= F^j\frac{\partial \xi^i}{\partial x^j}, && i,j=1,\dots,n,\\
\overline{w}^i &= -\frac{\partial \xi^i}{\partial t} = \frac{\partial x^j}{\partial \tau}\frac{\partial \xi^i}{\partial x^j}, && i,j=1,\dots,n.
\end{aligned}$$

For $\overline{A}_0^{ij}$ we obtain

$$\begin{aligned}
\overline{A}_0^{00} &= A^{00},\\
\overline{A}_0^{0i} &= A^{00}\frac{\partial \xi^i}{\partial t} + A^{0m}\frac{\partial \xi^i}{\partial x^m} = \overline{A}^{0i} - A^{00}\overline{w}^i, && i=1,\dots,n,\\
\overline{A}_0^{i0} &= \overline{A}^{i0} - A^{00}\overline{w}^i, && i=1,\dots,n,\\
\overline{A}_0^{ij} &= A^{00}\overline{w}^i\overline{w}^j - \overline{A}^{0j}\overline{w}^i - \overline{A}^{i0}\overline{w}^j + \overline{A}^{ij}, && i,j=1,\dots,n.
\end{aligned}$$

Analogously, for $\overline{\Gamma}^i_{kj}$ we obtain

$$\begin{aligned}
\overline{\Gamma}^0_{kj} &= 0, && k,j=0,1,\dots,n,\\
\overline{\Gamma}^i_{00} &= \frac{\partial \overline{w}^i}{\partial t} + \overline{w}^l\overline{w}^m\Gamma^i_{lm}, && i,l,m=1,\dots,n,\\
\overline{\Gamma}^i_{j0} &= \Gamma^i_{0j} = \frac{\partial \overline{w}^i}{\partial \xi^j} + \overline{w}^l\Gamma^i_{jl}, && i,j,l=1,\dots,n,\\
\overline{\Gamma}^i_{jk} &= \Gamma^i_{jk}, && i,j,k=1,\dots,n,
\end{aligned}$$

and for $\overline{F}^i_0$,

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