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# Note

## Numerical Divergence of a Tensor*

The finite-difference expressions which can be written to approximate a partial differential equation (to a given order) are not uniquely determined by the original partial differential equation. In three dimensions the divergence of a vector can be written as a six-point finite-difference function, i.e., a function of the six nearest neighbor points. This is true on any coordinate grid. The finite-difference expression for the divergence of a tensor is a six-point function on a Cartesian grid, but appears to be a seven-point function (involving the central point) on other grids. In some numerical schemes (such as leapfrog), each quantity is defined only on certain grid points. For example, if the tensor represents a flux through a cell wall, it may not be well defined at the cell center. To obtain the tensor at that point a spatial average can be performed. However, it is not clear how best to take an average of a tensor on a non-Cartesian grid. Alternatively, in a restricted class of leapfrog-type schemes a temporal average may be utilized.

For analytic work it is natural to choose derivatives and tensor or vector components in the same coordinate system. This leads to the seven-point function. The central term arises to cancel the effects of basis vectors whose direction is position dependent. We will show that for numerical work, a Cartesian basis for the uncontracted components of the tensor yields a six-point function which avoids the ambiguity created by the seven-point function. This technique is equivalent to choosing a particular technique for averaging a tensor on a non-Cartesian grid.

Before proceeding with a general proof, we illustrate the technique by discussing the divergence of both a vector and a tensor on a two-dimensional polar grid.

### Illustrations

For the divergence of a vector, it is straightforward to avoid the central (undifferentiated) terms. For example, consider a polar coordinate system. The non-zero elements of the metric tensor [1–4] are

$$g_{rr} = g^{rr} = 1, \qquad g_{\theta\theta} = r^2, \qquad g^{\theta\theta} = r^{-2},$$

giving

$$g \equiv g_{rr} g_{\theta\theta} = r^2.$$





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The physical component (denoted by an asterisk) as well as the covariant and contravariant components of vector **A** are related by [1]

$$A_r^* = A_r = A^r, \qquad A_\theta^* = A_\theta r^{-1} = A^\theta r.$$

The vector divergence is given by [1]

$$\nabla \cdot \mathbf{A} = \frac{\partial A^j}{\partial x^j} + \begin{Bmatrix} j \\ k\ j \end{Bmatrix} A^k, \tag{1}$$

where the Christoffel symbol is defined as

$$\begin{Bmatrix} \sigma \\ \mu\ \ \nu \end{Bmatrix} = \frac{1}{2} g^{\sigma\lambda} \left\{ \frac{\partial g_{\mu\lambda}}{\partial x^\nu} + \frac{\partial g_{\nu\lambda}}{\partial x^\mu} - \frac{\partial g_{\mu\nu}}{\partial x^\lambda} \right\}. \tag{2}$$

The Einstein summation convention is used here and throughout this paper. In polar coordinates the only nonzero Christoffel symbols are

$$\begin{Bmatrix} r \\ \theta\ \theta \end{Bmatrix} = -r, \qquad \begin{Bmatrix} \theta \\ r\ \theta \end{Bmatrix} = \begin{Bmatrix} \theta \\ \theta\ r \end{Bmatrix} = r^{-1}. \tag{3}$$

Thus (1) becomes

$$\nabla \cdot \mathbf{A} = \frac{\partial A^r}{\partial r} + \frac{\partial A^\theta}{\partial \theta} + \frac{A^r}{r}. \tag{4}$$

The last term, a nondifferentiated component, is the type we wish to avoid. In this case it can be readily avoided by rewriting (4) as

$$\nabla \cdot \mathbf{A} = \frac{1}{r} \frac{\partial}{\partial r} (rA^r) + \frac{\partial A^\theta}{\partial \theta} = \frac{1}{r} \frac{\partial}{\partial r} (rA_r^*) + \frac{1}{r} \frac{\partial}{\partial \theta} A_\theta^*, \tag{5}$$

which also comes from

$$\nabla \cdot \mathbf{A} = \frac{1}{g^{1/2}} \frac{\partial}{\partial x^j} (g^{1/2} A^j). \tag{6}$$

Both Eqs. (1) and (6) appear in the tensor analysis textbooks, and they are analytically equivalent. However the form of Eq. (6) leads more naturally to a six-point finite-difference expression, while Eq. (1) leads more naturally to a seven-point expression.

This simple device for incorporating nondifferentiated terms into an existing derivative term is not completely successful for tensors of rank 2 or higher. The divergence of a second rank tensor is given by [1]

$$(\nabla \cdot \mathbf{T})^i = T^{ji}_{,j} = \frac{\partial}{\partial x^j} T^{ji} + \begin{Bmatrix} j \\ k\ j \end{Bmatrix} T^{ki} + \begin{Bmatrix} i \\ k\ j \end{Bmatrix} T^{jk}. \tag{7}$$

Here the last two terms contain an undifferentiated tensor, and are therefore of the type we wish to eliminate. The first of these can be trivially incorporated into the derivative term as was done for the vector case. The last term requires the additional technique developed below.

To illustrate the technique, we choose polar coordinates and write the tensor as a dyadic

$$T^{ij} \equiv u^i v^j.$$

This gives

$$(\nabla \cdot \mathbf{T})_r^* = \frac{\partial}{\partial r}(u_r^* v_r^*) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_r^*) + \frac{1}{r} u_r^* v_r^* - \frac{1}{r} u_\theta^* v_\theta^*, \tag{8a}$$

$$(\nabla \cdot \mathbf{T})_\theta^* = r\frac{\partial}{\partial r}\left(\frac{1}{r} u_r^* v_\theta^*\right) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_\theta^*) + \frac{2}{r} u^* v_\theta^* + \frac{1}{r} u_\theta^* v_r^*. \tag{8b}$$

The third term in Eqs. (8a) and (8b) can be incorporated under a derivative, yielding

$$(\nabla \cdot \mathbf{T})_r^* = \frac{1}{r}\frac{\partial}{\partial r}(r u_r^* v_r^*) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_r^*) - \frac{1}{r} u_\theta^* v_\theta^*, \tag{9a}$$

$$(\nabla \cdot \mathbf{T})_\theta^* = \frac{1}{r}\frac{\partial}{\partial r}(r u_r^* v_\theta^*) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_\theta^*) + \frac{1}{r} u_\theta^* v_r^* . \tag{9b}$$

Strictly within the polar system it is not possible to incorporate the remaining terms. However, if we introduce Cartesian components for $v$

$$v_x \equiv v_r^* \cos\theta - v_\theta^* \sin\theta \tag{10a}$$

and

$$v_y \equiv v_r^* \sin\theta + v_\theta^* \cos\theta \tag{10b}$$

then

$$(\nabla \cdot \mathbf{T})_r^* = \cos\theta(\nabla \cdot \mathbf{T})_x + \sin\theta(\nabla \cdot \mathbf{T})_y \tag{11a}$$

and

$$(\nabla \cdot \mathbf{T})_\theta^* = -\sin\theta(\nabla \cdot \mathbf{T})_x + \cos\theta(\nabla \cdot \mathbf{T})_y , \tag{11b}$$

where

$$(\nabla \cdot \mathbf{T})_x = \frac{1}{r}\frac{\partial}{\partial r}(r u_r^* v_x) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_x) \tag{12a}$$

and

$$(\nabla \cdot \mathbf{T})_y = \frac{1}{r}\frac{\partial}{\partial r}(r u_r^* v_y) + \frac{1}{r}\frac{\partial}{\partial \theta}(u_\theta^* v_y). \tag{12b}$$

Equations (10)–(12) contain only differentiated expressions for $u$ and $v$; thus, if the derivatives in Eqs. (12) are expressed as centered differences, they achieve our stated objective. In those cases where $v$ and $\nabla \cdot T$ can be expressed throughout the problem in Cartesian components, Eqs. (10) and (11) are not necessary.

## Theorem and Proof

*The divergence of a tensor can always be written in an analytic form which leads to a six-point finite-difference expression on any three-dimensional grid.*

*Proof.* The divergence of a tensor of covariant rank $m$ and contravariant rank $n+1$ is given by [1]

$$T^{\alpha_0\alpha_1\cdots\alpha_n}_{\beta_1\cdots\beta_m,\alpha_0} = \frac{\partial}{\partial x^{\alpha_0}} T^{\alpha_0\cdots\alpha_n}_{\beta_1\cdots\beta_m} + \sum_{i=1}^{n} \begin{Bmatrix} \alpha_i \\ \gamma \quad \alpha_0 \end{Bmatrix} T^{\alpha_0\cdots\alpha_{i-1}\gamma\alpha_{i+1}\cdots\alpha_n}_{\beta_1\cdots\beta_m} - \sum_{j=1}^{m} \begin{Bmatrix} \delta \\ \beta_j \quad \alpha_0 \end{Bmatrix} T^{\alpha_0\cdots\alpha_n}_{\beta_1\cdots\beta_{j-1}\delta\beta_{j+1}\cdots\beta_m}. \tag{13}$$

Except for the first term, the right-hand side of Eq. (13) requires evaluating $T$ at the central point. To avoid this, one starts by transforming to Cartesian coordinates $\bar{x}^{y_i}$ and $\bar{x}^{z_i}$, where the bar denotes Cartesian space. If we let

$$S^{\alpha_1\cdots\alpha_n}_{\beta_1\cdots\beta_m} = T^{\alpha_0\cdots\alpha_n}_{\beta_1\cdots\beta_m\alpha,0}$$

then

$$S^{\alpha_1\cdots\alpha_n}_{\beta_1\cdots\beta_m} = \prod_{i=1,n} \frac{\partial x^{\alpha_i}}{\partial \bar{x}^{y_i}} \prod_{j=1,m} \frac{\partial \bar{x}^{z_j}}{\partial x^{\beta_j}} \bar{S}^{y_1\cdots y_n}_{z_1\cdots z_m},$$

where

$$\begin{aligned}
\bar{S}^{y_1\cdots y_n}_{z_1\cdots z_m} &= \frac{\partial}{\partial \bar{x}^{y_0}} \bar{T}^{y_0\cdots y_n}_{z_1\cdots z_m} \\
&= \frac{\partial x^{\alpha_0}}{\partial \bar{x}^{y_0}} \frac{\partial}{\partial x^{\alpha_0}} \left[ T^{\gamma_0\cdots\gamma_n}_{\delta_1\cdots\delta_m} \prod_{k=0,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \right] \\
&= \frac{\partial x^{\alpha_0}}{\partial \bar{x}^{y_0}} \frac{\partial \bar{x}^{y_0}}{\partial x^{\gamma_0}} \frac{\partial}{\partial x^{\alpha_0}} \left[ T^{\gamma_0\cdots\gamma_n}_{\delta_1\cdots\delta_m} \prod_{k=1,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \right] \\
&\quad + \frac{\partial x^{\alpha_0}}{\partial \bar{x}^{y_0}} T^{\gamma_0\cdots\gamma_n}_{\delta_1\cdots\delta_m} \prod_{k=1,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \frac{\partial}{\partial x^{\alpha_0}} \left( \frac{\partial \bar{x}^{y_0}}{\partial x^{\gamma_0}} \right) \\
&= \frac{\partial}{\partial x^{\gamma_0}} \left[ T^{\gamma_0\cdots\gamma_n}_{\delta_1\cdots\delta_m} \prod_{k=1,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \right] \\
&\quad + T^{\gamma_0\cdots\gamma_n}_{\delta_1\cdots\delta_m} \prod_{k=1,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \frac{\partial}{\partial \bar{x}^{y_0}} \left( \frac{\partial \bar{x}^{y_0}}{\partial x^{\gamma_0}} \right).
\end{aligned} \tag{14}$$

The final factor in the last term can be reexpressed by noting that the transformation law for Christoffel symbols is [1]

$$\left\{ {\sigma \atop \rho\ \tau} \right\} = \overline{\left\{ {i \atop j\ k} \right\}} \frac{\partial x^\sigma}{\partial \bar{x}^i} \frac{\partial \bar{x}^j}{\partial x^\rho} \frac{\partial \bar{x}^k}{\partial x^\tau} + \frac{\partial x^\sigma}{\partial \bar{x}^k} \frac{\partial}{\partial x^\rho} \left( \frac{\partial \bar{x}^k}{\partial x^\tau} \right). \tag{15}$$

But, if the $i, j, k$ are in Cartesian space, then $\overline{\{ {i \atop j\ k} \}} = 0$ and

$$\frac{\partial}{\partial \bar{x}^{y_0}} \left( \frac{\partial \bar{x}^{y_0}}{\partial x^{\gamma_0}} \right) = \left\{ {\tau \atop \tau\ \gamma_0} \right\} = \frac{1}{g^{1/2}} \frac{\partial}{\partial x^{\gamma_0}} g^{1/2}. \tag{16}$$

Therefore

$$\bar{S}^{y_1 \cdots y_n}_{z_1 \cdots z_m} = \frac{1}{g^{1/2}} \frac{\partial}{\partial x^{\gamma_0}} \left[ g^{1/2} \frac{\partial x^{\gamma_0}}{\partial \bar{x}^{y_0}} \bar{T}^{y_0 \cdots y_n}_{z_1 \cdots z_m} \right] \tag{17}$$

or

$$S^{\alpha_1 \cdots \alpha_n}_{\beta_1 \cdots \beta_m} = \prod_{i=1,n} \frac{\partial x^{\alpha_i}}{\partial \bar{x}^{y_i}} \prod_{j=1,m} \frac{\partial \bar{x}^{z_j}}{\partial x^{\beta_j}} \frac{1}{g^{1/2}} \frac{\partial}{\partial x^{\gamma_0}} \left[ g^{1/2} T^{\gamma_0 \cdots \gamma_n}_{\delta_1 \cdots \delta_m} \prod_{k=1,n} \frac{\partial \bar{x}^{y_k}}{\partial x^{\gamma_k}} \prod_{l=1,m} \frac{\partial x^{\delta_l}}{\partial \bar{x}^{z_l}} \right]. \tag{18}$$

In either case the divergence has been written as a sum of derivative terms.

## Conclusion

By the simple device of expressing the uncontracted components of a tensor in Cartesian components, a finite difference form for the divergence of a tensor can be written (Eq. (17) or (18)) as a six-point function. This function utilizes values of the tensor at the six nearest neighbor points, but not at the central point of the difference scheme. The technique, in the form of Eqs. (10)–(12), has proven useful in solving the ideal MHD equations in toroidal geometry [5] when applied to the stress tensor.

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## References

1. A. I. Borisenko and I. E. Tarapov, "Vector and Tensor Analysis with Applications," Prentice-Hall, Englewood Cliffs, N. J., 1968.
2. J. L. Synge and A. Schild, "Tensor Calculus," Univ. of Toronto Press, Toronto, 1964.

3. B. Spain, "Tensor Calculus," Oliver & Boyd, London, 1965.
4. J. Abram, "Tensor Calculus through Differential Geometry," Butterworths, London, 1965.
5. H. R. Hicks, G. Bateman, and D. N. Clark, *Bull. Amer. Phys. Soc.* **21**, 1080 (1976).

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H. R. Hicks
J. W. Wooten

*Computer Sciences Division*†
*Oak Ridge National Laboratory*
*Union Carbide Corporation*
*Nuclear Division*
*Oak Ridge, Tennessee 37830*

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