Differential operators for high-rank tensors in cylindrical and spherical coordinates

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1. Motivation and objectives

A high-order numerical framework for simulating the elastic-plastic deformation of materials with strength using a fully Eulerian discretization has been recently developed. The initial formulation of the method is discussed by Ghaisas et al. (2018), with the extension to multiple materials discussed by Subramaniam et al. (2018). The introduction of regularization to the kinematic equations is discussed by Adler & Lele (2019), and methods for interface regularization in multiphase settings are discussed by Adler et al. (2020) and Jain et al. (2020). The underlying numerical schemes follow the high-order framework of Cook (2007), and the treatment of multiple phases employs the four-equation, multicomponent model, with the pressure and temperature equilibration algorithm discussed by Cook (2009). The material-strength model requires the solution to kinematic equations that describe the evolution of inverse-deformation-gradient tensors. The total-inverse-deformation-gradient tensor is multiplicatively decomposed into two components that describe the elastic and plastic components of the deformation of the material, respectively. This strength model has been inspired by various sources, including Miller & Colella (2001), Favrie et al. (2009), and Ortega et al. (2014).

In many applications, the geometry of the problem of interest is better suited to discretization in cylindrical or spherical coordinates than to the heretofore implemented Cartesian discretization. However, unlike Cartesian coordinates, because the derivatives of the bases of these new coordinate systems with respect to one another are generally non-zero, the use of these new coordinates systems requires more complex forms for the differential operators needed for high-rank tensor operations. The inverse-deformation-gradient tensors are rank-two tensors to which various differential operators are applied in the kinematic equations. Some operations are comparatively simple, such as the application of an inner product to these rank-two tensors followed by calculation of the gradient of the resulting rank-one tensor. Other operations are more complex, including the calculation of the gradient of these rank-two tensors. The most involved operation is necessitated by the localized artificial diffusivity that acts to regularize these inverse-deformation-gradient tensors; this operation requires the calculation of the gradient of a rank-two tensor followed by the calculation of the divergence of a rank-three tensor.

Implementation of the differential operators for these high-rank tensors in non-trivial coordinate systems requires explicitly expanded expressions for the operators. Many documents on the subject of continuum mechanics discuss tensor calculus in cylindrical and spherical coordinates and include suitable expressions for operations on rank-one tensors (Reddy 2007) or rank-two tensors (Happel & Brenner 2012). However, we have not identified in the literature any satisfactory, explicitly expanded expressions for the divergence of rank-three tensors in these coordinates systems, although, compact notations for deriving such expressions are discussed (Hoffmann 2003). Furthermore, it is often

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inconvenient to have to reference the complete set of these expressions, which are from
different sources and represented by different notations. Therefore, this brief should serve
as a reference to the complete set of explicitly expanded expressions for these differential
operators for high-rank tensors when represented in non-trivial coordinate systems. All
of the results presented in this brief have been derived independently and subsequently
confirmed via symbolic algebraic manipulation software.

This brief is outlined as follows. Section 2 recaps the primary governing equations
and exposes the differential operators in the kinematic equations that require non-trivial
operator forms when represented in cylindrical and spherical coordinates. For complete-
ness, Section 3 explicitly expands the operators for the Cartesian representation and
should provide the opportunity for the reader to become familiar with our notation. Sec-
tion 4 explicitly expands the differential operators for the cylindrical representation, and
Section 5 explicitly expands the differential operators for the spherical representation.

2. Equations for material strength

2.1. Governing equations

The governing equations for the evolution of the multiphase flow or multimaterial con-
tinuum in conservative Eulerian form are

\[
\frac{\partial \rho Y_m}{\partial t} + \frac{\partial \rho u_k Y_m}{\partial x_k} = - \frac{\partial (J^*_m)}{\partial x_i} + \frac{J_m}{\partial x_i} \tag{2.1}
\]

\[
\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_k} \left( \rho \left( \epsilon + \frac{1}{2} u_j u_j \right) - u_i \sigma_{ik} \right) = \frac{\partial \tau^*_{ik}}{\partial x_k} + \frac{F_i}{\partial x_k} \tag{2.2}
\]

\[
\frac{\partial}{\partial t} \left[ \rho \left( \epsilon + \frac{1}{2} u_j u_j \right) \right] + \frac{\partial}{\partial x_i} \left[ u_k \rho \left( \epsilon + \frac{1}{2} u_j u_j \right) - u_i \sigma_{ik} \right] = \frac{\partial}{\partial x_k} \left( u_i \tau^*_{ik} - q^*_k \right) + \frac{H}{\partial x_k} \tag{2.3}
\]

which include the conservation of species mass [Eq. (2.1)], total momentum [Eq. (2.2)],
and total energy [Eq. (2.3)]. These are followed by the kinematic equations that track
material deformation,

\[
\frac{\partial g^e_{ij}}{\partial t} + \frac{\partial g^e_{ik} u_k}{\partial x_j} + u_k \left( \frac{\partial g^e_{ij}}{\partial x_k} - \frac{\partial g^e_{ik}}{\partial x_j} \right) = - \frac{1}{2 \mu \tau_{rel}} g^e_{ik} \sigma^\prime_{kj} + \frac{\zeta^e}{\Delta t} \left( \rho \frac{1}{\rho_0} - 1 \right) g^e_{ij} + \frac{\partial}{\partial x_k} \left( g^{\epsilon*} \frac{\partial g^e_{ij}}{\partial x_k} \right) + \frac{K^e_{ij}}{\partial x_k} \tag{2.4}
\]
High-rank differential operators

\[ \frac{\partial G^p_{ij}}{\partial t} + u_k \frac{\partial G^p_{ij}}{\partial x_k} + \frac{1}{2\mu_{rel}} \left( G^p_{kj} g^e_{kj} \sigma^i_{lm} (g^e)^{-1}_{ml} + G^p_{kj} g^{\epsilon}_{kj} \sigma^i_{ml} (g^e)^{-1}_{ml} \right) \]

local derivative  

advection  

elastic-plastic source

\[ = Z^p \left( \frac{1}{|G^p|^{1/2}} - 1 \right) G^p_{ij} + \frac{\partial}{\partial x_k} \left( G^p \frac{\partial G^p_{ij}}{\partial x_k} \right) \]

density compatibility  

artificial diffusion

\[ \frac{\partial g^e}{\partial t} + \nabla (g^e \cdot u) + \left( u \cdot \nabla g^e - (\nabla g^e) \cdot u \right) - \frac{1}{2\mu_{rel}} g^e \sigma^e \]

curl-free advection/strain  

non-zero curl advection/strain  

elastic-plastic source

\[ = \frac{\zeta^e}{\Delta t} \left( \frac{\rho}{\rho_0} g^e - 1 \right) g^e + \nabla \cdot (g^e \nabla g^e) + \frac{K^e}{\Delta t} \]

density compatibility  

artificial diffusion  

interface regularization

\[ \frac{\partial G^p}{\partial t} + u \cdot \nabla G^p + \frac{1}{2\mu_{rel}} \left( (g^e)^{-T} (\sigma^e)^T (g^e)^{-1} \right) G^p + \left( G^p \right)^T g^e \sigma^e (g^e)^{-1} \]

density compatibility  

artificial-plastic source

\[ = Z^p \left( \frac{1}{|G^p|^{1/2}} - 1 \right) G^p + \nabla \cdot (G^p \nabla G^p) \]

density compatibility  

artificial diffusion

which include the elastic component of the inverse deformation gradient tensor [Eq. (2.4)] and the symmetric Finger tensor [Eq. (2.5)] associated with plastic deformation. The kinematic equations are also presented in vector–tensor notation [Eqs. (2.6) and (2.7)].

Here, \( t \) and \( \mathbf{x} \) represent time and the Eulerian position vector, respectively. \( Y_m \) describes the mass fraction of each constituent material, \( m \). The variables \( u, \rho, \epsilon, \) and \( \mathbf{a} \) describe the mixture velocity, density, internal energy, and Cauchy stress, respectively, which are related to the species-specific components by the relations \( \rho = \sum_{m=1}^{M} \phi_m \rho_m, \epsilon = \sum_{m=1}^{M} Y_m \epsilon_m, \) and \( \mathbf{a} = \sum_{m=1}^{M} \phi_m \mathbf{a}_m \), in which \( \phi_m \) is the volume fraction of material \( m \), and \( M \) is the total number of material constituents.

The right-hand-side terms describe the localized artificial diffusion, including the artificial viscous stress, \( \tau^s_{ik} = 2\mu^* S_{ik} + (\beta^* - 2\mu^*/3) (\partial u_{ij}/\partial x_j) \delta_{ik} \), and the artificial enthalpy flux, \( q^e_i = -\kappa^* \partial T/\partial x_i + \sum_{m=1}^{M} h_m (J_m^e)_{ij} \), with temperature, \( T \), and strain rate tensor, \( S_{ik} = (\partial u_i/\partial x_k + \partial u_k/\partial x_i)/2 \). The second term in the artificial enthalpy flux expression is the enthalpy diffusion term (Cook 2009), in which \( h_m = \epsilon_m + p_m/\rho_m \) is the enthalpy of species \( m \). The artificial Fickian diffusion of species \( m \) is described by \( (J^e_m)_i = -\rho \left[ D^m_\epsilon \left( \partial Y_m/\partial x_i \right) - Y_m \sum_k D^e_k \left( \partial Y_k/\partial x_i \right) \right] \). In Eqs. (2.6) and (2.7), the boldface symbols without an underline denote vector quantities, and boldface symbols with an underline denote rank-two tensor quantities. A more complete discussion of the numerical framework can be found in the aforementioned references.

3. Operators in Cartesian coordinates

Consider a three-dimensional space with general coordinates \((x_i)\) and associated orthonormal basis vectors \((\hat{e}_i)\). The Cartesian coordinate system is described by coordinates
x = x₁, y = x₂, and z = x₃, in which x, y, and z represent the standard, orthogonal, Cartesian coordinates. The associated orthonormal basis vectors are, respectively, denoted by \( \hat{e}_x = \hat{e}_1 \), \( \hat{e}_y = \hat{e}_2 \), and \( \hat{e}_z = \hat{e}_3 \). Because the basis vectors are orthonormal, the inner product (\( \cdot \)) of any two basis vectors is the Kronecker delta with corresponding indices (\( \hat{e}_i \cdot \hat{e}_j = \delta_{ij} \)).

The Del operator may be described by

\[
\nabla = \hat{e}_i \frac{\partial}{\partial x_i} = \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z}.
\]

(3.1)

The partial derivatives of the basis vectors may be described by

\[
\frac{\partial \hat{e}_i}{\partial x_j} \hat{e}_j = \begin{pmatrix} \frac{\partial}{\partial x_1} \hat{e}_1 & \frac{\partial}{\partial x_1} \hat{e}_2 & \frac{\partial}{\partial x_1} \hat{e}_3 \\ \frac{\partial}{\partial x_2} \hat{e}_1 & \frac{\partial}{\partial x_2} \hat{e}_2 & \frac{\partial}{\partial x_2} \hat{e}_3 \\ \frac{\partial}{\partial x_3} \hat{e}_1 & \frac{\partial}{\partial x_3} \hat{e}_2 & \frac{\partial}{\partial x_3} \hat{e}_3 \end{pmatrix}
\]

(3.2)

As an example, for \( S_i = \delta_{ij} u_j \) (\( S = g^e \cdot u \)), the differential operator in the curl-free advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-one tensor, \( S = S_i \hat{e}_i \), becomes

\[
\nabla S \equiv \left( \hat{e}_i \frac{\partial}{\partial x_j} \right) (S_i \hat{e}_i) = \left( \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z} \right) (S_x \hat{e}_x + S_y \hat{e}_y + S_z \hat{e}_z)
\]

\[
= \frac{\partial S_x}{\partial x} \hat{e}_x \hat{e}_x + \frac{\partial S_y}{\partial y} \hat{e}_y \hat{e}_x + \frac{\partial S_z}{\partial z} \hat{e}_z \hat{e}_x + \frac{\partial S_x}{\partial y} \hat{e}_x \hat{e}_y \hat{e}_x + \frac{\partial S_y}{\partial z} \hat{e}_y \hat{e}_x \hat{e}_x + \frac{\partial S_z}{\partial x} \hat{e}_z \hat{e}_x \hat{e}_x
\]

\[
+ \frac{\partial S_x}{\partial z} \hat{e}_x \hat{e}_y \hat{e}_z + \frac{\partial S_y}{\partial x} \hat{e}_y \hat{e}_z \hat{e}_x + \frac{\partial S_z}{\partial y} \hat{e}_z \hat{e}_x \hat{e}_z.
\]

(3.3)

3.1. Gradient of a rank-one tensor

As an example, for \( S_{ij} = \delta_{ij} u_j \) (\( S = g^e \cdot u \)), the differential operator in the non-zero curl advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-two tensor, \( S = S_{ij} \hat{e}_i \hat{e}_j \), becomes

\[
\nabla S \equiv \left( \hat{e}_k \frac{\partial}{\partial x_k} \right) (S_{ij} \hat{e}_i \hat{e}_j) = \left( \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z} \right)
\]

\[
(S_{xx} \hat{e}_x \hat{e}_x + S_{xy} \hat{e}_x \hat{e}_y + S_{xz} \hat{e}_x \hat{e}_z
\]

\[
+ S_{yx} \hat{e}_y \hat{e}_x + S_{yy} \hat{e}_y \hat{e}_y + S_{yz} \hat{e}_y \hat{e}_z
\]

\[
+ S_{zx} \hat{e}_z \hat{e}_x + S_{zy} \hat{e}_z \hat{e}_y + S_{zz} \hat{e}_z \hat{e}_z).
\]

(3.4)
High-rank differential operators

\[
\frac{\partial S_{xx}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_x + \frac{\partial S_{xx}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_x + \frac{\partial S_{xx}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_x \\
+ \frac{\partial S_{xy}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_y + \frac{\partial S_{xy}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_y + \frac{\partial S_{xy}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_y \\
+ \frac{\partial S_{xz}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_z + \frac{\partial S_{xz}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_z + \frac{\partial S_{xz}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_z \\
+ \frac{\partial S_{yx}}{\partial x} \hat{e}_y \hat{e}_y \hat{e}_x + \frac{\partial S_{yx}}{\partial y} \hat{e}_y \hat{e}_y \hat{e}_y + \frac{\partial S_{yx}}{\partial z} \hat{e}_z \hat{e}_y \hat{e}_x \\
+ \frac{\partial S_{yy}}{\partial x} \hat{e}_y \hat{e}_y \hat{e}_y + \frac{\partial S_{yy}}{\partial y} \hat{e}_y \hat{e}_y \hat{e}_y + \frac{\partial S_{yy}}{\partial z} \hat{e}_z \hat{e}_y \hat{e}_y \\
+ \frac{\partial S_{yz}}{\partial x} \hat{e}_y \hat{e}_y \hat{e}_z + \frac{\partial S_{yz}}{\partial y} \hat{e}_y \hat{e}_y \hat{e}_z + \frac{\partial S_{yz}}{\partial z} \hat{e}_z \hat{e}_y \hat{e}_z \\
+ \frac{\partial S_{zx}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_z + \frac{\partial S_{zx}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_z + \frac{\partial S_{zx}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_z \\
+ \frac{\partial S_{zy}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_y + \frac{\partial S_{zy}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_y + \frac{\partial S_{zy}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_y \\
+ \frac{\partial S_{zz}}{\partial x} \hat{e}_x \hat{e}_x \hat{e}_z + \frac{\partial S_{zz}}{\partial y} \hat{e}_y \hat{e}_x \hat{e}_z + \frac{\partial S_{zz}}{\partial z} \hat{e}_z \hat{e}_x \hat{e}_z.
\]

3.3. Divergence of a rank-three tensor

As an example, for \( S_{ijk} = g^{ir} \frac{\partial \xi_j}{\partial x_i} (\mathbf{S} = g^{ie} \nabla g^e) \), the differential operator in the artificial diffusion term [Eq. (2.4) or (2.6)] involving the divergence of a rank-three tensor, \( \mathbf{S} \equiv S_{ij} \hat{e}_i \hat{e}_j \), becomes

\[
\nabla \cdot \mathbf{S} = \left( \hat{e}_i \frac{\partial}{\partial x_i} \right) \cdot (S_{ijk} \hat{e}_k \hat{e}_i \hat{e}_j) = \left( \hat{e}_x \frac{\partial}{\partial x} + \hat{e}_y \frac{\partial}{\partial y} + \hat{e}_z \frac{\partial}{\partial z} \right)
\cdot (S_{xxx} \hat{e}_x \hat{e}_x \hat{e}_x + S_{xxy} \hat{e}_x \hat{e}_x \hat{e}_y + S_{xxz} \hat{e}_x \hat{e}_x \hat{e}_z + S_{xyx} \hat{e}_x \hat{e}_y \hat{e}_x + S_{xyz} \hat{e}_x \hat{e}_y \hat{e}_y + S_{xyy} \hat{e}_x \hat{e}_y \hat{e}_z + S_{xyz} \hat{e}_x \hat{e}_y \hat{e}_z + S_{xzz} \hat{e}_x \hat{e}_z \hat{e}_z + S_{yxx} \hat{e}_y \hat{e}_x \hat{e}_x + S_{yxy} \hat{e}_y \hat{e}_x \hat{e}_y + S_{yyx} \hat{e}_y \hat{e}_x \hat{e}_z + S_{yyz} \hat{e}_y \hat{e}_y \hat{e}_x + S_{yzz} \hat{e}_y \hat{e}_y \hat{e}_z + S_{zxx} \hat{e}_z \hat{e}_x \hat{e}_x + S_{zxy} \hat{e}_z \hat{e}_x \hat{e}_y + S_{zyx} \hat{e}_z \hat{e}_x \hat{e}_z + S_{zxz} \hat{e}_z \hat{e}_x \hat{e}_z + S_{zyy} \hat{e}_z \hat{e}_y \hat{e}_x + S_{xyz} \hat{e}_z \hat{e}_y \hat{e}_z + S_{zyz} \hat{e}_z \hat{e}_y \hat{e}_z + S_{zzz} \hat{e}_z \hat{e}_z \hat{e}_z)
\]

\[
= \left( \frac{\partial S_{xxx}}{\partial x} + \frac{\partial S_{xxy}}{\partial y} + \frac{\partial S_{xxz}}{\partial z} \right) \hat{e}_x \hat{e}_x + \left( \frac{\partial S_{xyx}}{\partial x} + \frac{\partial S_{xyy}}{\partial y} + \frac{\partial S_{xyz}}{\partial z} \right) \hat{e}_x \hat{e}_y + \left( \frac{\partial S_{xyz}}{\partial x} + \frac{\partial S_{yxy}}{\partial y} + \frac{\partial S_{yyx}}{\partial z} \right) \hat{e}_y \hat{e}_x
\]

\[
+ \left( \frac{\partial S_{yxz}}{\partial x} + \frac{\partial S_{yyz}}{\partial y} + \frac{\partial S_{zxx}}{\partial z} \right) \hat{e}_z \hat{e}_x + \left( \frac{\partial S_{zyx}}{\partial x} + \frac{\partial S_{zyy}}{\partial y} + \frac{\partial S_{zxy}}{\partial z} \right) \hat{e}_z \hat{e}_y + \left( \frac{\partial S_{zyz}}{\partial x} + \frac{\partial S_{zzx}}{\partial y} + \frac{\partial S_{zyz}}{\partial z} \right) \hat{e}_z \hat{e}_z.
\]

(3.5)
Adler, West & Lele

4. Operators in cylindrical coordinates

4.1. Coordinate system definitions

Consider a three-dimensional space with general coordinates \((x_i)\) and associated orthonormal basis vectors \(\hat{e}_i\). The cylindrical coordinate system is described by coordinates \(r = x_1, \phi = x_2,\) and \(z = x_3\), in which \(r, \phi,\) and \(z\) represent the radial, azimuthal, and Cartesian-z coordinates. The associated orthonormal basis vectors are, respectively, denoted by \(\hat{e}_r = \hat{e}_1, \hat{e}_\phi = \hat{e}_2,\) and \(\hat{e}_z = \hat{e}_3\). Because the basis vectors are orthonormal, the inner product \(\langle \cdot, \cdot \rangle\) of any two basis vectors is the Kronecker delta with corresponding indices \(\langle \hat{e}_i, \hat{e}_j \rangle = \delta_{ij}\).

The Del operator may be described by

\[
\nabla \equiv \hat{e}_i \frac{\partial}{\partial x_i} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r} \frac{\partial}{\partial \phi} + \hat{e}_z \frac{\partial}{\partial z}.
\]

The partial derivatives of the basis vectors may be described by

\[
\frac{\partial \hat{e}_j}{\partial x_i} \hat{e}_j = \begin{pmatrix}
\frac{\partial}{\partial x_1} \hat{e}_1 & \frac{\partial}{\partial x_1} \hat{e}_2 & \frac{\partial}{\partial x_1} \hat{e}_3 \\
\frac{\partial}{\partial x_2} \hat{e}_1 & \frac{\partial}{\partial x_2} \hat{e}_2 & \frac{\partial}{\partial x_2} \hat{e}_3 \\
\frac{\partial}{\partial x_3} \hat{e}_1 & \frac{\partial}{\partial x_3} \hat{e}_2 & \frac{\partial}{\partial x_3} \hat{e}_3
\end{pmatrix}
= \begin{pmatrix}
0 & 0 & 0 \\
0 & \hat{e}_r & \hat{e}_\phi \\
0 & \hat{e}_z & 0
\end{pmatrix}.
\]

4.2. Gradient of a rank-one tensor

As an example, for \(S_i = \sigma_i^j u_j\) (\(S = g^e \cdot u\)), the differential operator in the curl-free advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-one tensor, \(\nabla \equiv S_i \hat{e}_i\), becomes

\[
\nabla S = \left( \hat{e}_i \frac{\partial}{\partial x_i} \right) (S_i \hat{e}_i) = \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r} \frac{\partial}{\partial \phi} + \hat{e}_z \frac{\partial}{\partial z} \right) (S_r \hat{e}_r + S_\phi \hat{e}_\phi + S_z \hat{e}_z)
\]

\[
= \frac{\partial S_r}{\partial r} \hat{e}_r \hat{e}_r + \frac{1}{r} \left( \frac{\partial S_r}{\partial \phi} - S_\phi \right) \hat{e}_\phi \hat{e}_r + \frac{\partial S_r}{\partial z} \hat{e}_z \hat{e}_r
+ \frac{\partial S_\phi}{\partial r} \hat{e}_r \hat{e}_\phi + \frac{1}{r} \left( \frac{\partial S_\phi}{\partial \phi} + S_r \right) \hat{e}_\phi \hat{e}_\phi
+ \frac{\partial S_\phi}{\partial z} \hat{e}_r \hat{e}_\phi
+ \frac{1}{r} \frac{\partial S_z}{\partial \phi} \hat{e}_\phi \hat{e}_z + \frac{\partial S_z}{\partial z} \hat{e}_z \hat{e}_z.
\]

4.3. Gradient of a rank-two tensor

As an example, for \(S_{ij} = \sigma_{ij}^e (S = g^e)\), the differential operator in the non-zero curl advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-two tensor, \(\nabla \equiv S_{ij} \hat{e}_i \hat{e}_j\), becomes
\( \nabla S = \left( \hat{e}_k \frac{\partial}{\partial x_k} \right) \left( S_{ij} \hat{e}_i \hat{e}_j \right) = \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r} \frac{\partial}{\partial \phi} + \hat{e}_z \frac{\partial}{\partial z} \right) \)

\[
\begin{align*}
S_{rr} \hat{e}_r \hat{e}_r &+ S_{r\phi} \hat{e}_r \hat{e}_\phi &+ S_{rz} \hat{e}_r \hat{e}_z \\
+ S_{\phi r} \hat{e}_\phi \hat{e}_r &+ S_{\phi \phi} \hat{e}_\phi \hat{e}_\phi &+ S_{\phi z} \hat{e}_\phi \hat{e}_z \\
+ S_{zr} \hat{e}_z \hat{e}_r &+ S_{z\phi} \hat{e}_\phi \hat{e}_z &+ S_{zz} \hat{e}_z \hat{e}_z \\
\end{align*}
\]

\[\frac{\partial S_{rr}}{\partial r} \hat{e}_r \hat{e}_r + \frac{1}{r} \left( \frac{\partial S_{rr}}{\partial \phi} - S_{r\phi} \right) \hat{e}_\phi \hat{e}_r \hat{e}_r &+ \frac{\partial S_{rr}}{\partial z} \hat{e}_z \hat{e}_r \\
+ \frac{\partial S_{r\phi}}{\partial r} \hat{e}_r \hat{e}_\phi &+ \frac{1}{r} \left( \frac{\partial S_{r\phi}}{\partial \phi} + S_{rr} - S_{\phi \phi} \right) \hat{e}_\phi \hat{e}_r \hat{e}_\phi &+ \frac{\partial S_{r\phi}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_\phi \\
+ \frac{\partial S_{rz}}{\partial r} \hat{e}_r \hat{e}_z &+ \frac{1}{r} \left( \frac{\partial S_{rz}}{\partial \phi} - S_{\phi z} \right) \hat{e}_\phi \hat{e}_r \hat{e}_z &+ \frac{\partial S_{rz}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_z \\
+ \frac{\partial S_{\phi r}}{\partial r} \hat{e}_r \hat{e}_\phi &+ \frac{1}{r} \left( \frac{\partial S_{\phi r}}{\partial \phi} + S_{rr} - S_{\phi \phi} \right) \hat{e}_\phi \hat{e}_r \hat{e}_r &+ \frac{\partial S_{\phi r}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_\phi \\
+ \frac{\partial S_{\phi \phi}}{\partial r} \hat{e}_r \hat{e}_\phi &+ \frac{1}{r} \left( \frac{\partial S_{\phi \phi}}{\partial \phi} + S_{\phi r} + S_{\phi \phi} \right) \hat{e}_\phi \hat{e}_r \hat{e}_\phi &+ \frac{\partial S_{\phi \phi}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_\phi \\
+ \frac{\partial S_{\phi z}}{\partial r} \hat{e}_r \hat{e}_z &+ \frac{1}{r} \left( \frac{\partial S_{\phi z}}{\partial \phi} + S_{zr} \right) \hat{e}_\phi \hat{e}_r \hat{e}_z &+ \frac{\partial S_{\phi z}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_\phi \\
+ \frac{\partial S_{zz}}{\partial r} \hat{e}_r \hat{e}_z &+ \frac{1}{r} \left( \frac{\partial S_{zz}}{\partial \phi} + S_{zz} \right) \hat{e}_\phi \hat{e}_r \hat{e}_z &+ \frac{\partial S_{zz}}{\partial z} \hat{e}_z \hat{e}_r \hat{e}_z.
\]

\[4.4\]

### 4.4. Divergence of a rank-three tensor

As an example, for \( S_{kij} = g^r e_i \frac{\partial}{\partial x_j} (S_{ij} e_j) \), the differential operator in the artificial diffusion term (Eq. (2.4) or (2.6)) involving the divergence of a rank-three tensor, \( \nabla \cdot \mathbf{S} \equiv S_{kij} \hat{e}_k \hat{e}_i \hat{e}_j \), becomes

\[\nabla \cdot \mathbf{S} = \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{1}{r} \frac{\partial}{\partial \phi} + \hat{e}_z \frac{\partial}{\partial z} \right) \]

\[
\cdot (S_{rrr} \hat{e}_r \hat{e}_r + S_{r\phi r} \hat{e}_r \hat{e}_\phi + S_{rzr} \hat{e}_r \hat{e}_z + S_{r\phi \phi} \hat{e}_r \hat{e}_\phi \hat{e}_\phi + S_{rz \phi} \hat{e}_r \hat{e}_z \hat{e}_\phi + S_{zzr} \hat{e}_r \hat{e}_z \hat{e}_z
\]

\[
+ S_{\phi r r} \hat{e}_\phi \hat{e}_r \hat{e}_r + S_{\phi \phi \phi} \hat{e}_\phi \hat{e}_\phi \hat{e}_\phi + S_{\phi z r} \hat{e}_\phi \hat{e}_z \hat{e}_r + S_{zz \phi} \hat{e}_\phi \hat{e}_z \hat{e}_\phi + S_{\phi \phi z} \hat{e}_\phi \hat{e}_\phi \hat{e}_z + S_{zzz} \hat{e}_\phi \hat{e}_z \hat{e}_z
\]

\[
+ S_{rzz} \hat{e}_r \hat{e}_z \hat{e}_r + S_{z\phi \phi} \hat{e}_\phi \hat{e}_\phi \hat{e}_\phi + S_{zzz} \hat{e}_\phi \hat{e}_z \hat{e}_z + S_{zz \phi} \hat{e}_\phi \hat{e}_z \hat{e}_\phi + S_{\phi \phi z} \hat{e}_\phi \hat{e}_\phi \hat{e}_z + S_{zzz} \hat{e}_\phi \hat{e}_z \hat{e}_z
\]

\[
+ S_{rzz} \hat{e}_r \hat{e}_z \hat{e}_r + S_{z\phi \phi} \hat{e}_\phi \hat{e}_\phi \hat{e}_\phi + S_{zzz} \hat{e}_\phi \hat{e}_z \hat{e}_z) \]

\[4.5\]
\[ \begin{align*}
\frac{\partial S_{rr}}{\partial r} + \frac{1}{r} \left( S_{rrr} + \frac{\partial S_{\phi r}}{\partial \phi} - S_{\phi r \phi} - S_{\phi \phi} \right) & \hat{e}_r \\
\frac{\partial S_{r \phi}}{\partial r} + \frac{1}{r} \left( S_{r \phi r} + S_{\phi r r} + \frac{\partial S_{\phi \phi}}{\partial \phi} - S_{\phi \phi \phi} \right) & \hat{e}_\phi \\\n\frac{\partial S_{zz}}{\partial z} & \hat{e}_z
\end{align*} \]

\[ \begin{align*}
\frac{\partial S_{r \phi}}{\partial \phi} + \frac{1}{r} \left( S_{r \phi \phi} + S_{\phi r \phi} + \frac{\partial S_{\phi \phi \phi}}{\partial \phi} \right) & \hat{e}_\phi \\
\frac{\partial S_{zz}}{\partial r} & \hat{e}_z
\end{align*} \]

\[ \begin{align*}
\frac{\partial S_{\phi \phi}}{\partial \phi} + \frac{1}{r} \left( S_{\phi \phi \phi} + S_{\phi \phi r} + \frac{\partial S_{\phi \phi \phi}}{\partial \phi} \right) & \hat{e}_{\phi \phi} \\
\frac{\partial S_{zz}}{\partial r} & \hat{e}_z
\end{align*} \]

5. Operators in spherical coordinates

5.1. Coordinate system definitions

Consider a three-dimensional space with general coordinates \((x_i)\) and associated orthonormal basis vectors \(\hat{e}_i\). The spherical coordinate system is described by coordinates \(r = x_1, \phi = x_2, \text{ and } \theta = x_3\), in which \(r, \phi, \text{ and } \theta\) represent the radial, polar, and azimuthal coordinates. The associated orthonormal basis vectors are, respectively, denoted by \(\hat{e}_r = \hat{e}_1, \hat{e}_\phi = \hat{e}_2, \text{ and } \hat{e}_\theta = \hat{e}_3\). Because the basis vectors are orthonormal, the inner product \((\cdot)\) of any two basis vectors is the Kronecker delta with corresponding indices \((\hat{e}_i \cdot \hat{e}_j = \delta_{ij})\).

The Del operator may be described by

\[ \nabla \equiv \hat{e}_i \frac{\partial}{\partial x_i} = \hat{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \hat{e}_\phi \frac{\partial}{\partial \phi} + \frac{1}{r \sin \theta} \hat{e}_\theta \frac{\partial}{\partial \theta}. \] (5.1)

The partial derivatives of the basis vectors may be described by

\[ \begin{align*}
\frac{\partial \hat{e}_i}{\partial x_j} \hat{e}_j & = \begin{pmatrix} \frac{\partial \hat{e}_1}{\partial x_1} & \frac{\partial \hat{e}_1}{\partial x_2} & \frac{\partial \hat{e}_1}{\partial x_3} \\ \frac{\partial \hat{e}_2}{\partial x_1} & \frac{\partial \hat{e}_2}{\partial x_2} & \frac{\partial \hat{e}_2}{\partial x_3} \\ \frac{\partial \hat{e}_3}{\partial x_1} & \frac{\partial \hat{e}_3}{\partial x_2} & \frac{\partial \hat{e}_3}{\partial x_3} \end{pmatrix} \\
& = \begin{pmatrix} \frac{\partial \hat{e}_r}{\partial \phi} & \frac{\partial \hat{e}_r}{\partial \theta} & \frac{\partial \hat{e}_r}{\partial \phi} \\ \frac{\partial \hat{e}_\phi}{\partial \phi} & \frac{\partial \hat{e}_\phi}{\partial \theta} & \frac{\partial \hat{e}_\phi}{\partial \phi} \\ \frac{\partial \hat{e}_\theta}{\partial \phi} & \frac{\partial \hat{e}_\theta}{\partial \theta} & \frac{\partial \hat{e}_\theta}{\partial \phi} \end{pmatrix} \begin{pmatrix} \delta_{ij} \\ \delta_{ij} \\ \delta_{ij} \end{pmatrix}.
\end{align*} \] (5.2)
5.2. Gradient of a rank-one tensor

As an example, for $S_i = g^e_i u_j$ ($S = g^e \cdot u$), the differential operator in the curl-free advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-one tensor, $S \equiv S_i \hat{e}_i$, becomes

$$\nabla S = \left[ \frac{\partial}{\partial x_j} \right] (S_i \hat{e}_i) = \left( \hat{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \hat{e}_\phi \frac{\partial}{\partial \phi} + \frac{1}{r \sin \phi} \hat{e}_\theta \frac{\partial}{\partial \theta} \right) \left( S_r \hat{e}_r + S_\phi \hat{e}_\phi + S_\theta \hat{e}_\theta \right)$$

(5.3)

5.3. Gradient of a rank-two tensor

As an example, for $S_{ij} = g^e_{ij}$ ($S = g^e$), the differential operator in the non-zero curl advection/strain term [Eq. (2.4) or (2.6)] involving the gradient of a rank-two tensor, $S \equiv S_{ij} \hat{e}_i \hat{e}_j$, becomes

$$\nabla S = \left[ \frac{\partial}{\partial x_k} \right] (S_{ij} \hat{e}_i \hat{e}_j) = \left( \hat{e}_r \frac{\partial}{\partial r} + \frac{1}{r} \hat{e}_\phi \frac{\partial}{\partial \phi} + \frac{1}{r \sin \phi} \hat{e}_\theta \frac{\partial}{\partial \theta} \right)$$

(5.4)
Adler, West & Lele

\[ + \frac{\partial S_{\phi\phi}}{\partial r} \hat{e}_r \hat{e}_\phi + \frac{1}{r} \left( \frac{\partial S_{\phi\phi}}{\partial \phi} + S_{r\phi} + S_{\phi r} \right) \hat{e}_\phi \hat{e}_\phi \]

\[ + \frac{1}{r} \left( \csc \phi \frac{\partial S_{\phi\theta}}{\partial \theta} - S_{\phi\theta} \cot \phi - S_{\theta\phi} \cot \phi \right) \hat{e}_\theta \hat{e}_\phi \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\phi\theta}}{\partial \phi} + S_{\theta\phi} \cot \phi + S_{\phi\phi} \right) \hat{e}_\phi \hat{e}_\theta \]

\[ + \frac{1}{r} \left( \csc \phi \frac{\partial S_{\phi\theta}}{\partial \theta} + S_{r\theta} + S_{\phi\theta} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\theta \hat{e}_r \]

\[ + \frac{1}{r} \left( \csc \phi \frac{\partial S_{\theta\phi}}{\partial \theta} + S_{\theta\theta} + S_{\theta\phi} \cot \phi - S_{\theta\theta} \cot \phi \right) \hat{e}_\phi \hat{e}_\theta \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\theta\phi}}{\partial \phi} - S_{\theta\theta} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\phi \hat{e}_\phi \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\theta\theta}}{\partial \phi} - S_{\theta\theta} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\phi \hat{e}_\theta \]

\[ + \frac{1}{r} \left( \csc \phi \frac{\partial S_{\theta\theta}}{\partial \theta} + S_{\theta\theta} + S_{\theta\phi} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\theta \hat{e}_\theta \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\theta\phi}}{\partial \theta} - S_{\theta\phi} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\theta \hat{e}_\phi \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\theta\phi}}{\partial \phi} - S_{\theta\phi} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\phi \hat{e}_\phi \]

\[ + \frac{1}{r} \left( \frac{\partial S_{\theta\theta}}{\partial \theta} - S_{\theta\theta} \cot \phi + S_{\theta\phi} \cot \phi \right) \hat{e}_\theta \hat{e}_\theta \]

\[ \equiv \nabla \cdot \mathbf{S} \equiv \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{\partial}{\partial \phi} + \hat{e}_\theta \frac{\partial}{\partial \theta} \right) \cdot \left( S_{kij} \hat{e}_k \hat{e}_j \right) = \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{\partial}{\partial \phi} + \hat{e}_\theta \frac{\partial}{\partial \theta} \right) \left[ \frac{\partial S_{rr}}{\partial r} + \frac{1}{r} \left( 2S_{rr} + \frac{\partial S_{\theta r}}{\partial \phi} + \cot \phi S_{\phi r} - S_{\phi r} + S_{\phi r} \right) \hat{e}_r \hat{e}_r \right. \]

\[ + \csc \phi \frac{\partial S_{\theta r}}{\partial \theta} - S_{\theta r} \right] \hat{e}_r \hat{e}_r \]

\[ + \left[ \frac{\partial S_{rr}}{\partial r} + \frac{1}{r} \left( 2S_{rr} + \frac{\partial S_{\theta r}}{\partial \phi} + \cot \phi S_{\phi r} - S_{\phi r} \right) \hat{e}_r \hat{e}_r \right. \]

\[ + \csc \phi \frac{\partial S_{\theta r}}{\partial \theta} - S_{\theta r} \right] \hat{e}_r \hat{e}_r \]

\[ \left( 5.5 \right) \]

5.4. Divergence of a rank-three tensor

As an example, for \( S_{kij} = g^{kr} \frac{\partial g_{rij}}{\partial x_k} \) (\( \mathbf{S} = g^{kr} \nabla g_{rij} \)), the differential operator in the artificial diffusion term [Eq. (2.4) or (2.6)] involving the divergence of a rank-three tensor, \( \mathbf{S} \equiv S_{kij} \hat{e}_k \hat{e}_i \hat{e}_j \), becomes

\[ \nabla \cdot \mathbf{S} \equiv \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{\partial}{\partial \phi} + \hat{e}_\theta \frac{\partial}{\partial \theta} \right) \cdot \left( S_{kij} \hat{e}_k \hat{e}_i \hat{e}_j \right) = \left( \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\phi \frac{\partial}{\partial \phi} + \hat{e}_\theta \frac{\partial}{\partial \theta} \right) \left[ \frac{\partial S_{rr}}{\partial r} + \frac{1}{r} \left( 2S_{rr} + \frac{\partial S_{\theta r}}{\partial \phi} + \cot \phi S_{\phi r} - S_{\phi r} + S_{\phi r} \right) \hat{e}_r \hat{e}_r \right. \]

\[ + \csc \phi \frac{\partial S_{\theta r}}{\partial \theta} - S_{\theta r} \right] \hat{e}_r \hat{e}_r \]

\[ + \left[ \frac{\partial S_{rr}}{\partial r} + \frac{1}{r} \left( 2S_{rr} + \frac{\partial S_{\theta r}}{\partial \phi} + \cot \phi S_{\phi r} - S_{\phi r} \right) \hat{e}_r \hat{e}_r \right. \]

\[ + \csc \phi \frac{\partial S_{\theta r}}{\partial \theta} - \cot \phi S_{\theta r} - S_{\theta r} \right] \hat{e}_r \hat{e}_r \]

\[ \left( 5.5 \right) \]
High-rank differential operators

\[ + \left[ \frac{\partial S_{rr\theta}}{\partial r} + \frac{1}{r} \left( 2S_{rr\theta} + \frac{\partial S_{\phi r\theta}}{\partial \phi} + \cot \phi S_{\phi r\theta} - S_{\phi \phi \theta} + S_{\theta rr} \right) \right] \hat{e}_r \hat{e}_\theta \\
+ \left[ \frac{\partial S_{r\phi r}}{\partial r} + \frac{1}{r} \left( 2S_{r\phi r} + \frac{\partial S_{\phi r}}{\partial \phi} + \cot \phi S_{\phi r} - S_{\phi \phi r} \right) \right] \hat{e}_\phi \hat{e}_r \\
+ \left[ \frac{\partial S_{\phi \phi r}}{\partial \theta} - S_{\phi \phi \theta} - \cot \phi S_{\theta \phi r} \right] \hat{e}_\phi \hat{e}_\theta \\
+ \left[ \frac{\partial S_{r\phi \theta}}{\partial r} + \frac{1}{r} \left( 2S_{r\phi \theta} + \frac{\partial S_{\phi \theta}}{\partial r} + \cot \phi S_{\phi \theta} - S_{\phi \phi \theta} + S_{\theta rr} \right) \right] \hat{e}_r \hat{e}_\phi \\
+ \left[ \frac{\partial S_{\theta \phi r}}{\partial \theta} + \cot \phi S_{\theta \phi r} + \csc \phi \frac{\partial S_{\theta \phi \theta}}{\partial \theta} \right] \hat{e}_\theta \hat{e}_r \\
+ \left[ \frac{\partial S_{\theta \phi \theta}}{\partial \theta} + \cot \phi S_{\theta \phi \theta} + \csc \phi \frac{\partial S_{\theta \theta \phi}}{\partial \theta} \right] \hat{e}_\theta \hat{e}_\phi \\
+ \left[ \frac{\partial S_{r\phi \theta}}{\partial r} + \frac{1}{r} \left( 2S_{r\phi \theta} + \frac{\partial S_{\theta \phi}}{\partial \phi} + \cot \phi S_{\theta \phi} - S_{\theta \phi \theta} + S_{\theta rr} \right) \right] \hat{e}_r \hat{e}_\phi. \]

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