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INVARIANTS OF $C^{1/2}$ IN TERMS OF THE INVARIANTS OF C

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The three invariants of $\boldsymbol{C}^{1/2}$ are key to expressing this tensor and its inverse as a polynomial in $\boldsymbol{C}$. Simple and symmetric expressions are presented connecting the two sets of invariants $\{I_1, I_2, I_3\}$ and $\{i_1, i_2, i_3\}$ of $\boldsymbol{C}$ and $\boldsymbol{C}^{1/2}$, respectively. The first result is a bivariate function relating I_1, I_2 to i_1, i_2. The functional form of i_1 is the same as that of i_2 when the roles of the $\boldsymbol{C}$-invariants are reversed. The second result expresses the invariants using a single function call. The two sets of expressions emphasize symmetries in the relations among these four invariants.

1. Introduction

We consider relations among the basic tensors of three dimensional continuum mechanics, all defined by the deformation $\boldsymbol{F}$,

$$\boldsymbol{F} = \boldsymbol{R}\boldsymbol{U} = \boldsymbol{V}\boldsymbol{R}, \qquad \boldsymbol{C} = \boldsymbol{F}^t\boldsymbol{F}, \qquad \boldsymbol{B} = \boldsymbol{F}\boldsymbol{F}^t.$$

$\boldsymbol{U}$ and $\boldsymbol{V}$ are symmetric and positive definite, and therefore

$$\boldsymbol{U} = \boldsymbol{C}^{1/2}, \qquad \boldsymbol{V} = \boldsymbol{B}^{1/2}.$$

Here we will only consider properties of $\boldsymbol{U}$ and $\boldsymbol{C}$, but the results apply to $\boldsymbol{V}$ and $\boldsymbol{B}$.

Although the square root of a second order positive definite symmetric tensor is unique and unambiguous it is not, however, a simple algebraic construct. One way to circumvent this problem is to express $\boldsymbol{U}$ as a polynomial in $\boldsymbol{C}$ using the Cayley–Hamilton equation,

$$\boldsymbol{U}^3 - i_1\boldsymbol{U}^2 + i_2\boldsymbol{U} - i_3\boldsymbol{I} = 0. \tag{1}$$

Here i_1, i_2, i_3 are the invariants of $\boldsymbol{U}$,

$$i_1 = \operatorname{tr}\boldsymbol{U}, \qquad i_2 = \frac{1}{2}(\operatorname{tr}\boldsymbol{U})^2 - \frac{1}{2}\operatorname{tr}\boldsymbol{U}^2, \qquad i_3 = \det\boldsymbol{U},$$

Multiply Equation (1) by $(\boldsymbol{U} + i_1\boldsymbol{I})$, and note that the result contains terms proportional to $\boldsymbol{I}$, $\boldsymbol{U}$, $\boldsymbol{U}^2$, and $\boldsymbol{U}^4$. Replacing the latter two by $\boldsymbol{C}$ and $\boldsymbol{C}^2$ gives [Ting 1985]

$$\boldsymbol{U} = (i_1i_2 - i_3)^{-1}\big(i_1i_3\boldsymbol{I} + (i_1^2 - i_2)\boldsymbol{C} - \boldsymbol{C}^2\big). \tag{2}$$

Note that $i_1i_2 - i_3 = \det(i_1\boldsymbol{I} - \boldsymbol{U}) > 0$ [Carroll 2004]. The inverse $\boldsymbol{U}^{-1}$ may be obtained by multiplying each side of Equation (2) with $\boldsymbol{C}^{-1}$ and using the Cayley–Hamilton equation for $\boldsymbol{C}$ to eliminate the single remaining $\boldsymbol{C}^{-1}$ term. The orthogonal rotation tensor follows as $\boldsymbol{R} = \boldsymbol{F}\boldsymbol{U}^{-1}$, from which one can determine kinematic quantities such as the rotation angle and the axis of rotation [Guan-Suo 1998].

Keywords: invariants, finite elasticity, stretch tensors, polar decomposition.

Equation (2) for $\boldsymbol{U}$ in terms of $\boldsymbol{C}$ avoids the tensor square root difficulty but introduces another: how to express $\{i_1, i_2, i_3\}$ in terms of $\boldsymbol{C}$, or more specifically, in terms of its invariants

$$I_1 = \operatorname{tr} \boldsymbol{C}, \qquad I_2 = \frac{1}{2}(\operatorname{tr} \boldsymbol{C})^2 - \frac{1}{2}\operatorname{tr} \boldsymbol{C}^2, \qquad I_3 = \det \boldsymbol{C}.$$

While the relation $i_3 = \sqrt{I_3}$ is simple, formulas for i_1 and i_2 are not. But as Equation (2) and related identities illustrate, the functional relations between the two sets of invariants are important for obtaining semiexplicit expressions for stretch and rotation tensors, and for their derivatives [Hoger and Carlson 1984b; Steigmann 2002; Carroll 2004].

The first such relations are due to Hoger and Carlson [1984a], who derived expressions for $\{i_1, i_2\}$ by solving a quartic equation. Sawyers [1986] subsequently showed that one can obtain alternative relations using the standard solutions [Goddard and Ledniczky 1997] for the cubic equation of the eigenvalue of $\boldsymbol{C}$. Let $\lambda_1, \lambda_2, \lambda_3$ be the (necessarily positive) eigenvalues of $\boldsymbol{U}$, then the eigenvalues of $\boldsymbol{C}$ are $\lambda_1^2, \lambda_2^2, \lambda_3^2$, and

$$i_1 = \lambda_1 + \lambda_2 + \lambda_3, \qquad i_2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1, \qquad i_3 = \lambda_1\lambda_2\lambda_3, \tag{3a}$$

$$I_1 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2, \qquad I_2 = \lambda_1^2\lambda_2^2 + \lambda_2^2\lambda_3^2 + \lambda_3^2\lambda_1^2, \qquad I_3 = \lambda_1^2\lambda_2^2\lambda_3^2. \tag{3b}$$

Sawyers' approach is to essentially compute the eigenvalues of $\boldsymbol{C}$, take their square roots and from these determine the invariants of $\boldsymbol{U}$ by Equation (3a). Jog [2006] generalized this scheme to tensors of order $n > 3$. This method does not provide direct relations between the invariants. Although the formulas of Hoger and Carlson [1984a] and of Sawyers [1986] are explicit, they are not totally satisfactory. In each case the functional forms are complicated. As we will see, there is no way to avoid this complexity since we are dealing with roots of cubic and quartic equations. But that is not the basic issue, rather it is a lack of any underlying symmetry or balance in the solutions of Hoger and Carlson [1984a] and of Sawyers [1986]. This makes it difficult to comprehend the formulas, and to place them in context. It is all the more unsettling by virtue of the fact that the formulas are associated with algebraic systems of deformation tensors, systems that are elegant and generally quite transparent.

The object of this paper is to express $\{i_1, i_2, i_3\}$ in terms of $\{I_1, I_2, I_3\}$ in two forms that each display the underlying symmetry of the relations. Both forms employ a single function, but have slightly different properties. We begin in section Section 2 with a summary of the principal results, followed by a review of the previously known solutions in Section 3. The new formulas for the invariants of $\boldsymbol{C}^{1/2}$ are derived in Section 4, with some closing comments in Section 5.

2. Principal results

Theorem 1. The invariants of $\boldsymbol{C}^{1/2}$ are

$$i_1 = I_3^{1/6} f\Big(\frac{I_1}{I_3^{1/3}}, \frac{I_2}{I_3^{2/3}}\Big), \qquad i_2 = I_3^{1/3} f\Big(\frac{I_2}{I_3^{2/3}}, \frac{I_1}{I_3^{1/3}}\Big), \qquad i_3 = I_3^{1/2}, \tag{4}$$

where f is a function of two variables,

$$f(x,y) = g(x,y) + \sqrt{x - g^2(x,y) + 2/g(x,y)}, \tag{5a}$$

$$g(x,y) = \Big(\frac{1}{3}\big(x + \sqrt{x^2-3y}\big[(\zeta+\sqrt{\zeta^2-1})^{1/3} + (\zeta-\sqrt{\zeta^2-1})^{1/3}\big]\big)\Big)^{1/2}, \tag{5b}$$

$$\zeta = \frac{27+2x^3-9xy}{2(x^2-3y)^{3/2}}. \tag{5c}$$

The function g can be expressed in the alternate form

$$g(x,y) = \sqrt{\frac{1}{3}\big(x + 2\sqrt{x^2-3y}\,\cos\big(\frac{1}{3}\arccos\zeta(x,y)\big)\big)}.$$

It is clear from Theorem 1 that the following reduced quantities are the important variables:

$$j_1 = \frac{i_1}{i_3^{1/3}}, \qquad j_2 = \frac{i_2}{i_3^{2/3}}, \tag{6a}$$

$$J_1 = \frac{I_1}{I_3^{1/3}}, \qquad J_2 = \frac{I_2}{I_3^{2/3}}, \tag{6b}$$

in terms of which the theorem states

$$j_1 = f(J_1, J_2), \qquad j_2 = f(J_2, J_1).$$

Alternatively, the sum and difference of reduced invariants may be considered as the key parameters, which is evident from:

Lemma 1. The following relation holds between the invariants of $\boldsymbol{C}$ and $\boldsymbol{C}^{1/2}$:

$$\frac{J_1 - J_2}{j_1 - j_2} = j_1 + j_2 + 2.$$

An immediate consequence is that we need only determine $j_1 + j_2$ or $j_1 - j_2$ since the other follows directly from Lemma 1. For instance, we could calculate $j_1 + j_2 = f(J_1, J_2) + f(J_2, J_1)$, but this requires evaluation of f twice, and it does not reveal the underlying symmetry of the arguments. The second result is a simpler relation between the invariants, one that uses a single call to the function f:

Theorem 2. The reduced invariants of $\boldsymbol{C}^{1/2}$ and $\boldsymbol{C}$ are connected by

$$j_1 = \frac{s}{2} + \frac{J_1 - J_2}{2s+4}, \tag{7a}$$

$$j_2 = \frac{s}{2} - \frac{J_1 - J_2}{2s+4}, \tag{7b}$$

where $s = s(J_1, J_2)$ is

$$s = (2 + J_1 + J_2)^{1/3}\, f\Big(\frac{6 + J_1 + J_2}{(2+J_1+J_2)^{2/3}}, \frac{9 + 5J_1 + 5J_2 + J_1J_2}{(2+J_1+J_2)^{4/3}}\Big). \tag{7c}$$

Thus $j_1 + j_2 = s(J_1, J_2)$, and s is a symmetric function of its arguments $s(x, y) = s(y, x)$. Also, s provides an alternative expression for the function f:

$$f(x, y) = \frac{1}{2}s(x, y) + \frac{x - y}{2s(x, y) + 4}.$$

This form for f employs the function itself, but evaluated at different arguments. This is a property of the nonlinear nature of the function.

3. The methods of Hoger and Carlson and of Sawyers

Starting from the identities Equation (3) it may be easily verified that [Hoger and Carlson 1984a]

$$i_1^2 - 2i_2 = I_1, \tag{8a}$$

$$i_2^2 - 2i_1 i_3 = I_2, \tag{8b}$$

$$i_3^2 = I_3. \tag{8c}$$

Equation (8c) implies $i_3 = I_3^{1/2}$. It remains to find i_1 and i_2.

Hoger and Carlson [1984a] eliminated i_2 between Equation (8a) and (8b) to obtain a quartic equation in i_i which they then solved. The same solution for i_i is obtained more directly by starting with the *ansatz*

$$i_i = \lambda + \rho, \tag{9}$$

where λ is any one of the triplet $\{\lambda_1, \lambda_2, \lambda_3\}$. For instance, if $\lambda = \lambda_1$ then $\rho = \lambda_2 + \lambda_3$ and $i_2 = \lambda_1(\lambda_2 + \lambda_3) + \lambda_2\lambda_3$ is

$$i_2 = \rho\lambda + i_3/\lambda. \tag{10}$$

This holds no matter which value λ takes. Substituting from Equation (9) into Equation (8a) implies

$$\rho^2 = I_1 - \lambda^2 + 2i_3/\lambda. \tag{11}$$

The right member is necessarily positive, and using $i_3 = I_3^{1/2}$ we can therefore express $\rho > 0$ in terms of I_1, I_3 and λ.

In summary,

$$i_1 = \lambda + \sqrt{I_1 - \lambda^2 + 2\sqrt{I_3}/\lambda}, \tag{12a}$$

$$i_2 = \sqrt{I_3}/\lambda + \sqrt{I_1\lambda^2 - \lambda^4 + 2\sqrt{I_3}\lambda}, \tag{12b}$$

$$i_3 = \sqrt{I_3}, \tag{12c}$$

where λ is any positive root of the characteristic equation of $\boldsymbol{C}$,

$$\lambda^6 - I_1\lambda^4 + I_2\lambda^2 - I_3 = 0. \tag{13}$$

For instance,

$$\lambda = \left(\frac{1}{3}(I_1 + [\xi + \sqrt{\xi^2 - (I_1^2 - 3I_2)^3}]^{1/3} + [\xi - \sqrt{\xi^2 - (I_1^2 - 3I_2)^3}]^{1/3})\right)^{1/2},$$

and

$$\xi = \frac{1}{2}(2I_1^3 - 9I_1 I_2 + 27I_3).$$

Note that we assumed that λ in Equations (9) and (10) is a root of (13), but this is actually a requirement, as can be seen from Equations (8) using (9)–(11). Equations (9) and (10) represent a standard method of reducing a quartic to a cubic equation.

Equation (12a) is essentially the same as the first relation of Hoger and Carlson [1984a, Equation (5.5)], although they did not identify the root of the cubic explicitly. It should be noted that the second relation in their Equation (5.5) never applies, because it can be shown that the equality cannot occur. Hoger and Carlson [1984a] recommended using Equation (8b) to obtain i_2. The relation (12b) is quite different and is suggestive of the symmetry underlying the solutions for i_1 and i_2 that is evident in Theorem 1. We discuss this further in the next section from a different perspective.

It is interesting to compare this with the explicit positive solution of Equation (13) provided by Guan-Suo [1998], based on [Sawyers 1986]. Starting with the characteristic equation for $\boldsymbol{U}$,

$$\lambda^3 - i_1\lambda^2 + i_2\lambda - i_3 = 0, \tag{14}$$

combined with Equation (8b) and Equation (8c), this becomes a quadratic equation for i_2. The solution is [Guan-Suo 1998, p. 199]

$$i_2 = \lambda^{-1}\big(\sqrt{I_3} + \sqrt{2\sqrt{I_3}\lambda^3 + I_2\lambda^2 - I_3}\big).$$

This appears to be different than Equation (12b), but they are equivalent when one takes into account that λ satisfies (13).

In short, Hoger and Carlson [1984a] and Sawyers [1986] derived Equation (12a) and (12b), respectively. They did not however note the symmetry between the formulas, which is one of the central themes in this paper: that a single function determines both i_1 and i_2. In the next section we complete the proof of Theorem 1.

4. An alternative approach

The three conditions in Equation (8) can be combined into a single polynomial identity,

$$(1 - i_2 z^2)^2 + (i_1 z - i_3 z^3)^2 = 1 + I_1 z^2 + I_2 z^4 + I_3 z^6, \qquad \text{for all } z \in \mathbb{C}.$$

Using the reduced variables of Equation (6), this becomes

$$(1 - j_2 z^2)^2 + (j_1 z - z^3)^2 = 1 + J_1 z^2 + J_2 z^4 + z^6, \qquad \text{for all } z \in \mathbb{C}.$$

Comparing coefficients implies the pair of coupled equations

$$j_1^2 - 2j_2 = J_1, \tag{15a}$$

$$j_2^2 - 2j_1 = J_2. \tag{15b}$$

Thus, solutions must be of the form

$$j_1 = f(J_1, J_2), \qquad j_2 = f(J_2, J_1),$$

for some function $f(x, y)$ which satisfies

$$f^2(x, y) - 2f(y, x) - x = 0. \tag{16}$$

This is the fundamental equation for $f(x, y)$. It implies the dual relation

$$f^2(y, x) - 2f(x, y) - y = 0. \tag{17}$$

Eliminating $f(y, x)$ leads to a quartic in $f = f(x, y)$:

$$(f^2 - x)^2 - 8f - 4y = 0. \tag{18}$$

This is equivalent to the quartic of [Hoger and Carlson 1984a] but expressed in the reduced variables. We have already derived a solution of the quartic in the previous section by using the ansatz of Equation (9) based on a root of the cubic (13). (12a) therefore *defines* the function f, which can be read off by converting to the reduced variables j_1, j_2, J_1, J_2. It may be easily verified that the function of (5) results.

But what about the relation (12b) for i_2? It does not seem to convert into the expression claimed in Theorem 1, that is, $j_2 = f(J_2, J_1)$. Rather, using (12b) and $j_2 = f(J_2, J_1)$ to define f we obtain a different expression for f:

$$f(y, x) = \frac{1}{g(x, y)} + \sqrt{x - g^2(x, y) + 2/g(x, y)}\, g(x, y). \tag{19}$$

This is, in fact, consistent with the definition of f in Theorem 1 because $g(x, y)$ satisfies the normalized version of (14),

$$g^3(x, y) - f(x, y)g^2(x, y) + f(y, x)g(x, y) - 1 = 0. \tag{20}$$

Using this and the expression for $f(x, y)$ in Equation (5), gives (19). This completes the proof of Theorem 1.

It is interesting to note from Equation (20) that $1/g(y, x)$ satisfies the same equations as $g(x, y)$, that is,

$$g^{-3}(y, x) - f(x, y)g^{-2}(y, x) + f(y, x)g^{-1}(y, x) - 1 = 0.$$

But this does not mean that $g(y, x)$ equals $1/g(x, y)$, since they can (and do) correspond to different roots of the cubic.

The identity in Lemma 1 follows from the coupled equations (15), and the details of the proof of Theorem 2 are in the Appendix.

5. Conclusion

Although the expressions for i_1 and i_2 involve the roots of the characteristic cubic equation of $\boldsymbol{C}$, it seems that the governing quartic Equation (18) is more fundamental. This is the equation that defines the functions f and s of Theorems 1 and 2. In fact s is defined by f, which is in some ways the central function involved. It is interesting that the quartic equation first considered by Hoger and Carlson [1984a] reappears in this manner.

Which of the expressions for i_1 and i_2 are actually best in practice? While the expressions in Equation (7) are perhaps the most aesthetically pleasing in form, (4) is probably simpler to implement. The final choice is of course left to the reader.

Appendix A. Proof of Theorem 2

For simplicity of notation, let f and f' denote $f(x, y)$ and $f(y, x)$, respectively. Then the coupled Equation (16) and (17) are

$$f^2 - 2f' = x,$$
$$f'^2 - 2f = y.$$

Adding and subtracting yields, respectively,

$$(f + f' - 1)^2 = 1 + x + y + 2ff',$$
$$(f - f')(f + f' + 2) = x - y,$$

which in turn imply

$$f + f' = s,$$
$$f - f' = \frac{x-y}{s+2},$$

where $s = 1 + \sqrt{1 + x + y + 2ff'}$. The function $s = s(x, y)$ is clearly a symmetric function of x and y, that is, it is unchanged if the arguments are switched.

Solving the linear equations for f and f' gives

$$f = \frac{s}{2} + \frac{x-y}{2s+4},$$
$$f' = \frac{s}{2} - \frac{x-y}{2s+4}.$$

Although these formulas clearly split f into parts that are symmetric and asymmetric in the two arguments, they are not explicit since the function s involves the product ff'. Taking the product of the two expressions leads to an equation for ff'. It is simpler to consider the equation for s, which after some manipulation may be reduced to the quartic:

$$[s^2 - (6 + x + y)]^2 - 8(2 + x + y)s - 4[(5 + x)(5 + y) - 16] = 0.$$

Let $s = (2 + x + y)^{1/3} u$; then u satisfies $(u^2 - X)^2 - 8u - 4Y = 0$, where

$$X = \frac{6 + x + y}{(2 + x + y)^{2/3}}, \qquad Y = \frac{9 + 5x + 5y + xy}{(2 + x + y)^{4/3}}.$$

The quartic equation for u is the same as the quartic Equation (18) satisfied by f, but with X and Y instead of x and y. Thus,

$$u = f(X, Y),$$

which completes the proof of Theorem 2.

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